# Remote Sensing of Grassland Variables Across Seasons and Using Multiple Spectral Devices

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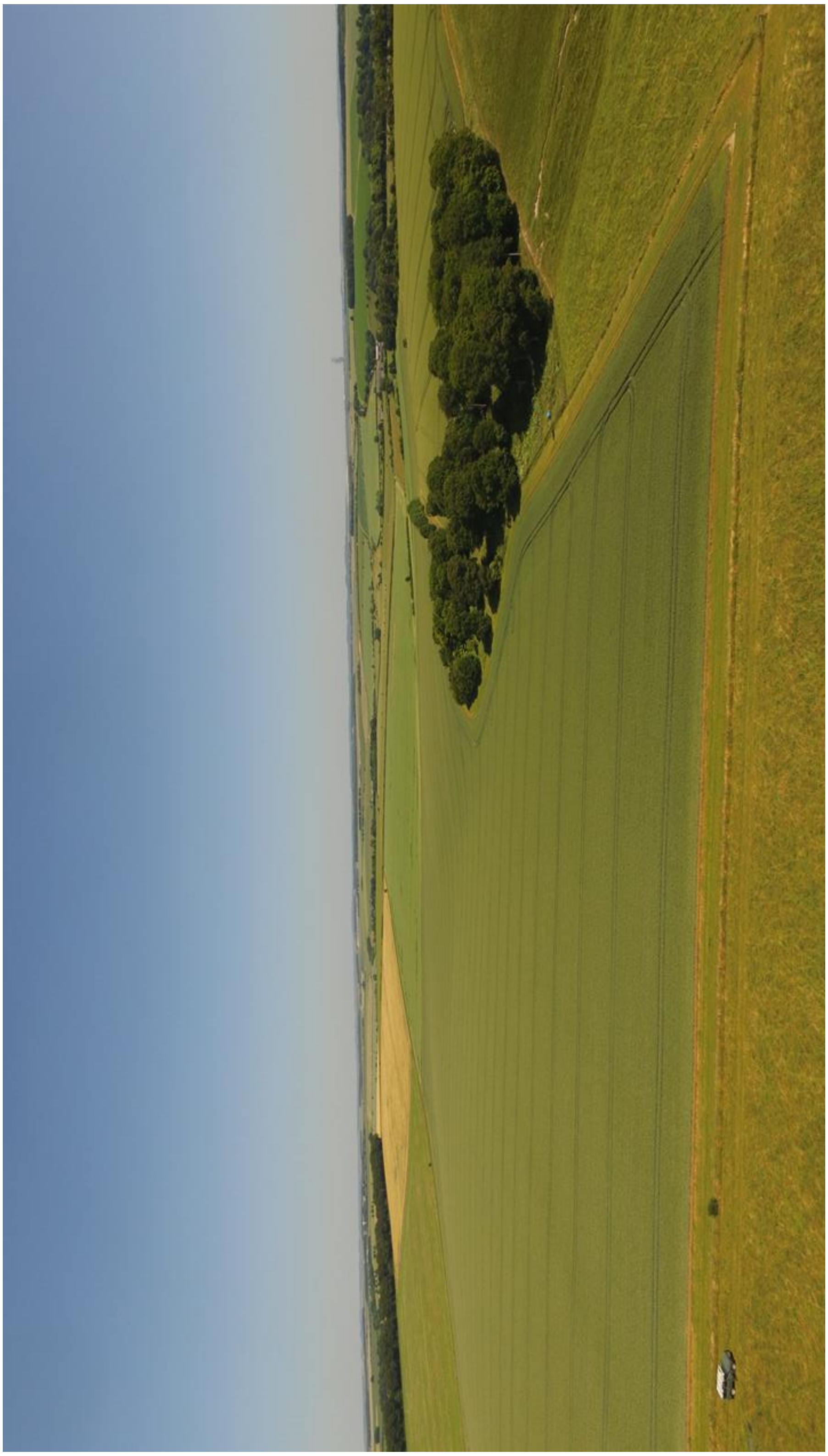
ROTHAMSTED RESEARCH



“Success is the ability to go from one failure to another without loss of enthusiasm.”

Winston Churchill

# Declaration

This thesis has not been submitted in support of an application for another degree at this or any other university. It is the result of my own work and includes nothing that is the outcome of work done in collaboration except where indicated. Many of the ideas in this thesis were the product of discussions with my supervisory team and other collaborators; Dr. France Gerard, Prof. Alan Blackburn, Mr. Charles George, Prof. Paul Harris, Dr. Douglas Kelley, and Dr. Simon Smart.

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# Abstract

In the UK, the regeneration and conservation of semi-natural grasslands is important, especially for grasslands protected by legislation such as UK Biodiversity Action Plan (BAP) priority habitats or Sites of Special Scientific Interest (SSSIs). As such, monitoring grassland condition is necessary, but conventional methods of measuring grassland condition are time consuming and limited in their spatial coverage. This thesis tested if remote sensing can provide a more cost- and time-effective solution to measuring grassland condition as defined by the Common Standards Monitoring (CSM).

A field spectroscopy experiment was designed to explore the potential link between grassland spectral reflectance, plus a metric representing a traditional measure of grassland condition referred to as CSM-condition. Partial least squares regressions were used to evaluate the relationship between grassland multi-spectral reflectance and a range of condition-related grassland variables; between the condition related grassland variables and CSM-condition and between the grassland multi-spectral reflectance and CSM-condition. The evaluation tested the relationships across grassland types, seasons and spectral devices used; and between grassland variable observations made in terms of mass or % cover.

When analysing data collected at patch level during the summer; the mass of bryophytes, dead material and graminoids plus the % cover of forbs can be predicted to a moderate level of accuracy ($R^2$ values of >0.5 and nRMSE <100) when analysing data from all seven grasslands. When analysing data from all Parsonage Down NNR grasslands; the mass of bryophytes, the % cover of live material, % cover-based live:dead ratio and CSM-condition could be predicted to a high level of accuracy ($R^2$ values of >0.7 and nRMSE <100). Moisture content plus the % cover of dead material, forbs and gram:forb ratio were all predicted to a moderate level of accuracy as well as CSM-condition predicted by grassland variable values. When using data from all Ingleborough NNR grasslands; the % cover of forbs and biomass plus the mass of bryophytes, dead material and live material could be predicted to a moderate level of accuracy. When using patch level data collected across three seasons; the % cover of dead material, live material and live:dead ratio plus the mass of graminoids could be predicted when using three seasons of data collected on one grassland, or for all three Parsonage grasslands, to at least a moderate level of accuracy although

some models trained with % cover data had a high accuracy. Forbs (mass and % cover) plus the mass of gram:forb ratio, live material and live:dead ratio could be predicted to at least a moderate level of accuracy for some grasslands.

When using data from all grasslands collected in one season the mass of a range of grassland variables could be predicted to a moderate level of accuracy for the spring and autumn months but not when using % cover data. Using CROPSCAN and SVC data produced similar results, with slightly stronger results from the CROPSCAN, but using data from the Rikola camera produced weaker results. When the results of trained PLSR models were extrapolated to field level, the projected predicted grassland variable values from models trained with CROPSCAN MSR 16R data looked promising but the results have not been externally validated using a separate data set. The most important spectral bands for predicting grassland variables and CSM-condition were NIR and SWIR with the red edge (647nm) and 470nm also having some importance. The most important grassland variables for predicting CSM-condition were depended on whether the grassland variable was mass-based or % cover-based. When using mass data; graminoid:forb ratio mass and live:dead ratio mass were consistently important. When using % cover data; forbs cover, graminoids cover and live:dead ratio cover were consistently important.

Overall, the results suggest that some of the condition-related variables considered in this thesis are predicted with reasonable accuracy and precision at patch level (i.e. R2 values of >0.5 and nRMSE <100), but producing reliable results requires a sufficient quantity of data to train the statistical models (at least 30 quadrats of samples), particularly if the results are to be extrapolated to field level as additional data are required for the external validation of the results. Grassland variable prediction success varied with number of sites considered and with season with no clear consistent pattern. Also, none of the grassland variables could be consistently predicted strongly across all the different grasslands or seasons.

This has implications for any land manager who wishes to emulate the methods in this thesis. The results suggest that this thesis provides a more cost- and time-effective solution for capturing grassland condition; but anyone emulating these methods would have to carefully choose the variables, grassland types and seasons to collect data and would have to collect a sufficient quantity of data for model training, testing and evaluation. A consequence of adopting, or refining, the approach in this thesis could be more effective monitoring (and therefore timely intervention where necessary) of UK Biodiversity Action Plan (BAP) priority habitats and Sites of

Special Scientific Interest (SSSIs). Refining this approach could include testing different modelling approaches and focusing further work on the successful aspects of this research such as key grassland and wavelength variables.

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# Abbreviations, Acronyms and Notations

ASD - Analytical Spectral Device

BAP - Biodiversity Action Plan

CSM – Common Standards Monitoring

CV - Coefficient of variation

EM - Electromagnetic spectrum

ENVI - Environmental Visualisation software

ES – Ecosystem service(s)

EVI - Enhanced vegetation index

EWT – Equivalent water thickness

FAPAR - Fraction of absorbed photosynthetically active radiation

FOV - Field of view

GAI – Green area index

JNCC - Joint Nature Conservation Committee

LAI - Leaf area index

LDMC – Leaf dry matter content

LWC - Leaf water content (%)

MODIS - Moderate Resolution Imaging Spectroradiometer

NDVI – Normalised difference vegetation index

NDWI – Normalised difference water index

NIR - Near infrared spectral domain (701-1400nm)

NNR - National Nature Reserve

nm - Nanometre

nRMSE - Normalised root mean square error

NVC - National Vegetation Classification

OLS - Ordinary Least Squares Regression

PCA - Principal component analysis

PAI – Plant area index

PLSR - Partial least squares regression

RE - Red edge spectral region (650-810nm)

RMSE - Root mean square error

RS - Remote sensing

SLA – Specific leaf area

SPOT - *Satellite Pour l'Observation de la Terre*

SSSI - Site of Special Scientific Interest

SVC - Spectra Vista Corporation

SWIR - Shortwave infrared spectral domain (1401-2500nm)

VIP - Variable importance of prediction

VIs - Vegetation indices

VIS - Visible spectral region (390-700nm)

VNIR - Visible to near infrared regions of the electromagnetic spectrum

VSWIR - Visible to shortwave infrared regions of the electromagnetic spectrum

# Chapter 1 - Introduction

## 1.1. Background

A report by the Food and Agricultural Organisation highlights the global extent of grasslands and their socio-economic importance. For example, an estimated one billion people depend on livestock as a source of income and food including approximately 70% of the world's rural poor (Neely et al., 2009). Despite their importance; grasslands face encroachment, degradation and fragmentation due to increasing population, urbanisation and industrial development (Reid et al., 2005). Grasslands are also subject to degradation or loss through overgrazing, intensive management practices and climate change (Ali et al., 2016; Bullock et al., 2011; Möckel et al., 2014; Neely et al., 2009). Grassland degradation results in reduced ecosystem services, increased carbon emissions, increased soil erosion, increased fertiliser use, increased likelihood of eutrophication of adjacent water bodies and biodiversity loss (Bullock et al., 2011; Dusseux et al., 2014; Möckel et al., 2014; Neely et al., 2009; Smith et al., 2009; Smith et al., 2016).

Although the loss in extent of semi-natural grasslands has slowed over the last ten years in the UK, agricultural improvement since 1945 has resulted in the loss of approximately 90% of semi-natural grasslands. This loss, primarily attributed to agricultural improvement through arable crop planting or fertiliser use, has caused a reduction in the wide range of ecological and recreational services that grasslands offer. Relative to agriculturally improved land, the services that semi-natural grasslands offer include reduced emissions of methane and nitrous oxide, improved effectiveness as a carbon sink, improved water infiltration and storage plus improved species richness with the ecosystem services that increased biodiversity offers. As part of the effort to preserve these ecosystem services, 2% of UK grassland areas were designated a Biodiversity Action Plan (BAP) priority habitat for their high biodiversity (Bullock et al., 2011) which has since been encompassed in the UK Post-2010 Biodiversity Framework (JNCC and DEFRA 2012).

For the purpose of facilitating grassland regeneration and conservation, this research was conducted within the context of providing landowners with a framework (Xu and Guo, 2015) to create spatial-temporal data analysis projections that provide cost- and time-effective grassland condition information. Such a framework would provide landowners with the means to identify impending land management issues and facilitate effective intervention. In addition, improved condition monitoring is considered particularly important in the UK, especially if predictions that farmlands will need to be worked more intensely and/or sustainably in the future become reality (Baulcombe et al., 2009; Garnett and Godfray, 2012; Godfray and Garnett, 2014; Pywell et al., 2015). There are few studies that directly attempt to understand how the remote sensing (RS) of grassland condition on semi-natural grasslands can be achieved as they often focus on experimental and/or relatively structurally homogeneous grasslands.

## 1.2. Research aims

The primary aim of this research is to assess the link between condition-related grassland variables (including a metric referred to as CSM-condition, explained in Section 3.4.1) with grassland spectral reflectance through field and drone spectro-radiometry at a range of spatial-temporal scales. The focus of achieving this aim is on grassland condition within the context of ecosystem services (ES) and on a range of grassland types that exist within the UK. thesis is focused on how RS techniques could be deployed to address some of the limitations of establishing grassland condition using traditional techniques by addressed the following questions:

1. Can grassland condition-related variables form the basis for RS-based approaches to monitoring grassland condition? Which grassland variables are the most suitable and are they suitable for all different types of grasslands?

2. Can grassland condition be determined accurately across seasons using remote sensing techniques?

3. Is it possible to upscale models trained with field radiometry data from patch level ($1m^2$) to field level using data collected with a CROPSCAN or a UAV?

Related to these are the following detailed questions:

4. Can PLSR models trained using spectral reflectance data predict grassland variables or CSM-condition with an acceptable level of accuracy (i.e. $R^2$>0.5

and nRMSE<100)? Can CSM-condition be predicted with an acceptable level of accuracy using grassland variable data?

5. Will using mass or % cover of grassland variables impact on the relationship between grassland variables and spectral reflectance?

6. Does utilising reflectance data recorded across a wider spectral range (i.e. including SWIR spectral values), instead of across the visible and near-infrared (NIR) spectrum, lead to more successful monitoring of grassland condition using remote sensing?

7. Does the choice of radiometry instruments affect the relationship between grassland variables and reflectance?

8. Which spectral reflectance bands are the strongest predictors of each grassland variable including CSM-condition and which grassland variables are the strongest predictors of CSM-condition?

# 1.3. Thesis structure

This thesis is presented according to the requirements to attain a PhD at Lancaster University and consists of eight chapters. Chapter 1 (this chapter) introduces the thesis, including the research context and research aims. Chapter 2 provides a literature review that encompasses many approaches to establishing grassland condition, both conventional and by using RS methods. Chapter 3 describes and discusses the research methods. This includes a detailed description of sampling strategy and the analytical processes applied to captured data sets.

There are three main chapters to this thesis which have been summarised in Figure 1.1, all of which explore particular aspects of the RS of grassland condition. Chapter 4 investigates the ability to predict condition-related grassland variables on seven semi-natural grasslands; three grasslands at Parsonage Down NNR and four grasslands at Ingleborough NNR using data collected in summer. This work directly addresses issues around conducting RS studies of grassland condition on a range of different types of structurally heterogeneous semi-natural grasslands. Chapter 5 investigates the relationship between reflectance and condition-related grassland variables across the growing seasons, focussing on the three sites at Parsonage Down NNR. This work directly addresses questions regarding which time of the year is most effective for collecting data to calibrate a PLSR model that will have the most predictive power, or whether calibrating a PLSR with data from three seasons gives it more predictive power than using data collected from just one season. The results of Chapters 4 and 5 raised questions about the importance of different regions of the EM spectrum in predicting grassland variables. Chapter 6 investigates the value of SWIR data by comparing the predictive power of different PLSR models trained with reflectance spectra from three different spectral devices that collect spectral data in slightly different spectral regions, numbers of bands and spectral resolution. As this research would only be useful to landowners if results could be upscaled to field level, Chapter 6 also explores the ability of PLSR models trained with data collected at patch level ($1m^2$) to predict grassland variable values at field level (200x1m). Chapter 7 discusses the results presented in the previous three chapters. Chapter 8 concludes the thesis by providing key findings, potential future research plus considerations that should be taken when using the methods described in this thesis.

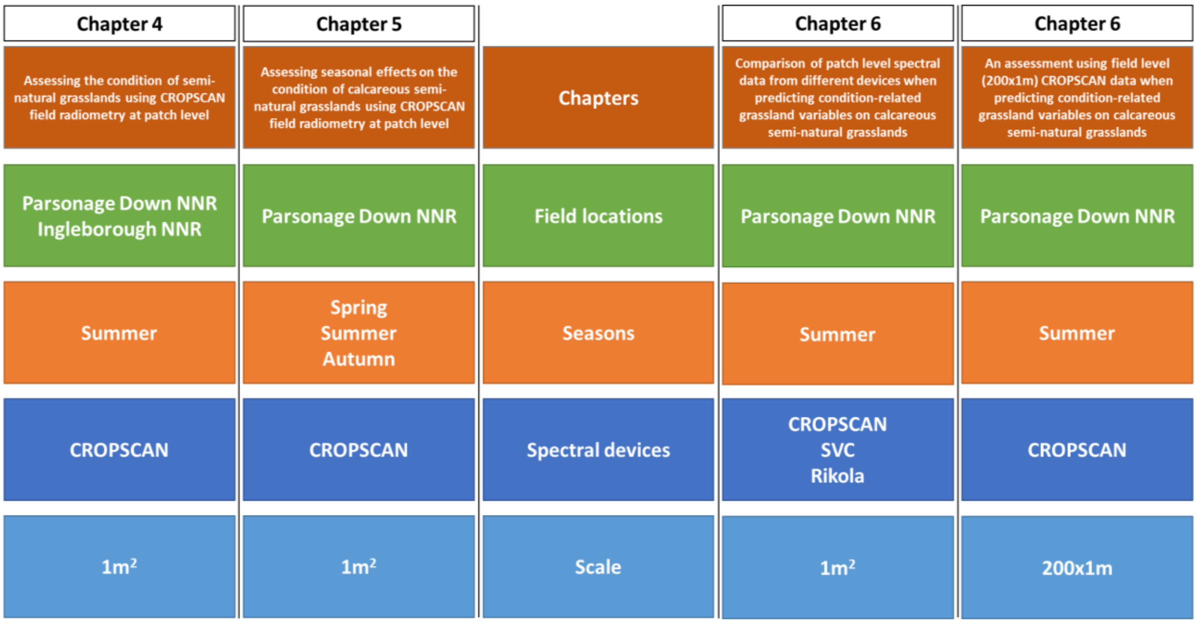



*Figure 1.1: Schematic of the attributes of each of the main chapters of this thesis, highlighting how the thesis chapters are different from each other.*

# Chapter 2 - Literature Review

## 2.1. The conventional approach to measuring grassland condition *in situ*

The term “grassland condition” has multiple interpretations, which will influence the metrics used to define it. For land managers such as commercial farmers, grassland condition may refer to grassland productivity, grass nutrient content or the number of grazing animals that can be supported (Badgery et al., 2020; Bullock et al., 2011; Marsett et al., 2006; Schils et al., 2013). A report by Schils et al. (2013) explains that a range of destructive and non-destructive methods (including RS techniques) can be used to quantify grassland productivity. Broadly speaking; conventional methods of productivity measurements focusses on dry matter yield, grassland density or just grassland height. Grassland productivity can also be indirectly quantified by quantifying animal products or the number of grazing animals, e.g. by quantifying fodder milk units or fodder units intensive beef production. Other studies may use linked grassland variables such as biomass to estimate productivity. For example, Ni (2004) used destructive sampling to estimate biomass and then used modelling techniques to estimate net primary productivity (using biomass and other variables such as climate) on a range of grasslands in northern China. Fliervoet (1987) used grass cuttings to establish biomass and leaf area index on fifteen different grassland types in Holland. These grasslands were then divided into four different levels of productivity using data collected on leaf size and inclination in a principal components analysis. Bai et al. (2001) used grass cuttings, ruler measurements of grass height, % cover estimates of grassland variables and % cover estimates of species abundance to quantify multiple grassland variables and then used these variables to examine the relationship between biodiversity, productivity and herbivory. First, species biomass data were used to quantify grassland condition where grassland condition refers to productivity. Then, the link between condition and the height, mass and/or % cover of the following grassland variables was assessed using canonical correspondence analysis (CCA): biomass, live material, graminoids, forbs, bryophytes, dead material and bare soil. One conclusion of the study was that an increase in quantity in all of these variables except the bryophyte-based variables and bare soil was linked with better grassland condition in relation to better productivity.

Other land managers, particularly those who have a legal obligation to protect or improve the ecosystem services (ES) value of the grasslands that they manage, may instead consider grassland condition from this perspective (Bullock et al., 2011). Ecosystem services are broadly defined as a range of goods and services provided by nature and these services can be categorised as provisioning services (e.g. food), regulating services (e.g. flood control), cultural services (e.g. recreation) or supporting services which refers to any services that supports the other three categories such as nutrient cycling (Lamarque et al., 2011). Studies on ecosystem services usually focus on a specific aspect of this broad remit (Plantureux et al., 2016). The main focal points of these studies according to Rodríguez-Ortega et al. (2014) are gene pool protection (including biodiversity), climate regulation (including carbon sequestration) and also grassland aesthetic value (including cultural value). Zhao et al. (2020) stated that carbon sequestration, preventing water erosion of the soil and above-ground biomass (productivity) are the most frequently mentioned ecosystem services in the 380 papers and 32 book chapters that were reviewed but 33 different ecosystem services were mentioned at least once.

Some authors linked different ecosystem services by showing that some ecosystem services can have a positive impact on others, referred to as complementarity. Tilman et al. (2006) conducted a decade-long study on experimental grasslands and found that ecosystem stability (and therefore the provision of ecosystem services including productivity) improved with increased biodiversity. Craven et al. (2016) conducted a meta-analysis using data collected on 16 grasslands across North America and Europe to assess whether more biodiverse grasslands are more resilient to the negative effects of fertilisation and drought regarding their ecosystem service value. This study was conducted in the context that greater biodiversity increases the functioning of ecosystems. It was found that the positive effects of biodiversity on above-ground productivity are robust to the effects of fertilisation and drought. Reich et al. (2012), using two experimental grasslands for data collection including the Cedar Creek experiment used by Tilman et al. (2006), found that the negative impact of biodiversity loss on biomass and productivity becomes greater over time.

In the EU, some areas that provide ecosystem services such as biodiversity, aesthetic or recreational value are chosen to become part of the Natura 2000 network of conservation sites. This includes some types of grasslands which can be designated as special areas of conservation (SACs) and as special protection areas (SPAs) if threatened bird species inhabit them. For example, grasslands labelled as

"(6210) semi-natural dry grasslands and scrubland facies on calcareous substrates (*Festuco-Brometalia*)" are a part of the Natura 2000 network because of their relatively high plant biodiversity, their recreational value and also because of their protected bird and Orchid species. Each classification of grassland has a system of conservation and monitoring specific to it, which takes into consideration the biggest threats to those grasslands. For example, some of the biggest threats to the aforementioned *Festuco-Brometalia* grasslands are related to natural afforestation and therefore a focal point of the overall strategy for monitoring and conservation is the prevention of shrub species from succeeding over grass species. Monitoring of these grasslands to ensure that the management strategy is working focuses on plant species counts, although these species counts can be expanded to include insect and bird species (Calaciura and Spinelli, 2008; Silva et al. 2008).

Within the context of ecosystem services in the UK, the conventional approach to monitoring grassland condition is detailed in the Common Standards Monitoring (CSM) guidance with National Vegetation Classification (NVC) standards being provided for each classified grassland type. The NVC standards recommend identifying grassland communities primarily using species abundance data and information on environmental variables. CSM guidance discusses the use of a number of generic primary and secondary attributes (or criteria), plus some criteria specific to each NVC grassland type, as a means of establishing grassland condition. Primary attributes refer to characteristics chosen for community identification whilst secondary attributes relate to sward structure; height, litter and bare ground. Secondary attributes are highly variable and easily reversible through cutting or grazing and are therefore considered less reliable than primary attributes (JNCC, 2004; 2006).

The primary attributes consist of grass:herb ratio (a.k.a. graminoid:forb ratio), grassland extent, positive and negative indicator species plus other indicators of local distinctiveness such as transitional zonation and rare species. Diversity and productivity are considered too time consuming to be regularly or effectively monitored, hence indicator species are chosen as primary attributes (JNCC, 2004). Noss (1990) warned that focusing on indicator species alone may prevent the discovery of some environmental trends, which may explain why CSM guidance also includes other criteria such as environmental variables. Grasslands that do not meet the criteria specific to their NVC category are considered to be in unfavourable condition (JNCC, 2004; 2006).

Although the studies discussed in this section generally did not use RS techniques, they provide evidence that there is a link between some ecosystem services such as biomass, productivity and biodiversity. A RS of grassland condition study still requires some data gathering on condition-related grassland variables which requires a fieldwork campaign (see Figure 2.1) even if collecting these data is time consuming and limited in its spatial coverage. Furthermore, the CSM guidelines make assumptions about which criteria best reflect grassland condition and how effective they are at capturing changes in condition over space and time.

*Figure 2.1: Conventional grassland data being collected on a quadrat at Over Pasture (Ingleborough NNR).*

## 2.2. Remote sensing platforms used in grassland condition studies

Studies investigating the use of RS for grassland condition primarily used devices mounted on UAVs or satellites, sometimes in conjunction with hand-held devices and destructive samples, with relatively few studies exclusively using hand-held devices or using devices mounted on crewed aircraft. The wide variety of devices deployed is reflected in the range of spatial scales used in these studies, which ranged from leaf level to regional level. There are also several considerations to make when deploying spectral devices. Readings can be taken at nadir only (e.g. Schile et al., 2013) or multiple directions (e.g. Cole et al., 2014). Some devices have a dual field of view, where readings can be taken of incoming radiation as well as the target. These devices can display or utilise downwelling illumination readings, making it easier to make an informed decision on whether the illumination is adequate for RS data collection, and may automatically calculate reflectance values of the target based on downwelling illumination. Readings taken in low illumination conditions can lead to a reduced signal to noise ratio, especially in the SWIR part of the spectrum (Roelofsen et al., 2014) and electro-optical satellite imagery can be obscured by clouds. Therefore, it is common practice to collect data with spectral devices in clear sky conditions and within two hours of solar maximum (e.g. Guo et al., 2005; Yao et al., 2013) as solar zenith angle can have an impact on results (Ishihara et al., 2015) or to choose satellite imagery with as little cloud cover as possible. Even when spectral data are collected in clear sky conditions, short-term changes in irradiance and atmospheric conditions will affect the observed spectral data. The only way to account for this is by converting readings into reflectance. This requires concurrent observations of downwelling (i.e. irradiance) and upwelling radiation (i.e. reflected radiance) or measurements taken intermittently between the target (such as vegetation) and a reference calibration panel (Dusseux et al., 2014). Drone or crewed aircraft imagery collected across areas which include reference panels placed on the ground, and collected in conjunction with other ground-based spectral devices, can achieve the same purpose.

Within the context of grassland condition, each device and supporting platform has advantages and disadvantages relative to others when taking into consideration important aspects such as spatial resolution, spatial coverage and spectral information. Table 2.1 summarises the comparison between the main types of platforms used to support spectral devices; the main types of platforms being hand-held, uncrewed aerial vehicles (UAVs), crewed aircraft and satellites. There is an overlap in some metrics between platforms, for example the most expensive and heaviest hand-held devices (e.g. ASD FieldSpec Pro) can be more expensive and heavier than the cheapest and lightest drones (e.g. DJI Parrot), and the most expensive and heaviest aircraft (e.g. NASA Ikhana drone) can be more expensive and heavier than the cheapest and lightest satellites (e.g. Dove nanosatellites by Planet Labs Inc.).

Table 2.1: Overview of widely available RS platforms

| **System** | **No of spectral bands** | **Spatial resolution** | **Repeat frequency** | **Spatial coverage** | **Flight time** | **Portability** | **Government regulations** | **Size of team** | **Platform cost** | **Image cost to customer** |
|---|---|---|---|---|---|---|---|---|---|---|
| Satellite | Few-multi spectral<br><br>RGB, NIR, SWIR, TIR | Low to very high (km - cm) | 1-16 days, determined by satellite orbit and constellation number | From global to user defined ~10,000 $km^2$ areas | Years | N/A | N/A | Very high | Very high | Free to very high |
| Crewed aircraft | Few-hyperspectral<br><br>RGB, NIR, SWIR | High (meters) | Single or more repeat visits determined by user | < 10,000 $km^2$ | Hours | Low | High | High | High-very high | Free to high |
| UAS | Few-multi spectral<br><br>RGB & NIR | High-very high (m-cm) | Single or more repeat visits determined by user | meters-hectares | Minutes -hours | Low-high | High | Low-high | Low-high | Free to high |
| Hand-held | Few-hyperspectral<br><br>RGB, NIR, SWIR | High-very high (m-cm) | Single or more repeat visits determined by user | Samples of <5$m^2$ | N/A | High | Low | Low | Low-med | N/A |

Relative to other platforms; the strongest advantages of using hand-held devices are their portability and, in the case of devices such as the Analytical Spectral Device FieldSpec Pro (referred to as ASD from now on), their ability to collect hyperspectral data along a relatively wider range of the electromagnetic (EM) spectrum. One of the biggest disadvantages of hand-held devices is their reduced spatial coverage over most UAVs, aircraft or satellite imagery as they can only take spot measurements. Anderson and Gaston (2013) and Von Beuren et al. (2015) explored the advantages and disadvantages of UAV data collection compared to other platforms. Despite small drone-mounted cameras having less functionality, for example because these devices collect data on fewer spectral wavelengths, they are much more flexible to deploy making it easier to collect data at a higher spatial-temporal resolution than crewed aircraft or satellites. UAV platforms are also becoming more cost effective and therefore more accessible. Spatial coverage, which varies subject to the size of the UAV (Anderson and Gaston, 2013), is improved when compared to using hand-held devices but not when compared to crewed aircraft (except for the largest UAVs or satellite imagery). UAV-mounted multi-spectral cameras are generally limited to the visible and NIR part of the EM spectrum and are expensive. Although aircraft have the advantage of rapidly collecting hyperspectral imagery over a relatively large area, crewed aircraft have much greater asset, maintenance and storage costs plus asset deployment is more challenging. Furthermore, with the exception of the largest UAVs and satellites, a greater quantity and expertise of crew is required for operations. Satellite mounted sensors can collect relatively large swaths of imagery anywhere on Earth including regions that may be inaccessible due to terrain or conflict (Geerken et al., 2005). Also, some optical sensors cover a relatively wide region of the EM spectrum (e.g. Landsat-8 covers VIS to TIR range of EM spectrum) although satellites generally use broader bands than hand-held devices. Furthermore, satellite imagery from government-owned satellites are often made freely and easily accessible to the general public but access to commercial imagery can be costly. Satellite data generally have a low spectral and spatial resolution compared to data from hand-held devices and drone-mounted cameras (Lillesand et al., 2015) and the number of available spectral bands is predetermined and limited when compared to hyperspectral hand-held devices and UAV-mounted multi spectral devices.

### 2.2.1. Field radiometry (hand-held spectral devices)

Field radiometry studies that use hand-held devices have been used in proof of concept studies plus these data are often used for the purpose of calibrating or evaluating satellite, aircraft or UAV derived data products. Within the context of vegetation condition studies, hand-held devices such as the CROPSCAN MSR 16R or ASD FieldSpec Pro have been used to collect reflectance data on different vegetation types (e.g. Dusseux et al., 2014), bare soil and litter (Asner et al., 2000) or lichens and exposed rock (Veen et al., 2006). Data may be collected on target patches in the field or on samples (such as leaf cuttings) in a laboratory (e.g. Asner, 1998). Within the context of grassland condition studies, spectral data from hand-held devices have been collected for calibration purposes or to utilise as predictors of above ground biomass (Psomas et al., 2011), biochemical variables (e.g. nitrogen content) ( Roelofsen et al. 2014; Polley et al. 2022), vegetation indices (e.g. Yang and Guo, 2014) or a combination of at least some of the aforementioned categories of variables (Asner, 1998; Asner et al., 2000).

Relative to each other; hand-held devices can also offer very different spectral ranges, spectral coverage, spatial coverage and portability. Hyperspectral devices such as the ASD provide superior spectral range (350-2500nm), spectral coverage (data collected on most wavelengths in this range) and spectral resolution (bandwidths of 3nm) but are expensive. On the other hand, data collection with a CROPSCAN MSR 16R is easy relative to devices such as the ASD FieldSpec Pro and SVC HR-1024i as these devices need regular calibration whilst the CROPSCAN MSR 16R collects upwelling and downwelling radiation simultaneously. Furthermore, the CROPSCAN MSR 16R is relatively lightweight, portable and robust with a longer battery life making it relatively quick and easy to collect data in the field.

### 2.2.2. Uncrewed Aerial Vehicles (UAV) and crewed aircraft remote sensing

Anderson and Gaston (2013) described the four main categories of UAV platform which are primarily delineated by size: large UAVs (payload ~200-1100kg), medium (payload ~50kg), small and mini (payload ~5-30kg), and micro and nano (payload <5kg). Larger UAVs have the advantages of being able to carry a larger payload, fly to a higher altitude and have a longer flight time. On the other hand, larger drones have higher running and setup costs. Larger drones also have greater logistical challenges such as asset storage and operation (Anderson and Gaston, 2013). The same advantages and disadvantages of using a large UAV also applies to using crewed aircraft.

*Figure 2.2: A custom-built Matrice 600 UAV being prepared for launch at Scar Close Moss at Ingleborough NNR.*

UAV-mounted sensors are being utilised for environmental monitoring in a wide variety of applications including grassland condition (see review by Salamí et al., 2014). UAV RS of grassland condition studies usually focus on particular grassland variables (particularly biomass, e.g. Capolupo et al. (2015)) but can include biochemical variables (e.g. Polley et al. 2022) and species composition (e.g. Lu et al., 2009) which usually includes the deployment of small rotary drones (<10kg). Small drone platforms are becoming increasingly common in RS studies.  Although UAV based RS studies have become more commonplace since 2015, replacing crewed aircraft-based RS studies, organisations such as the Natural Environment Research Council Airborne Research Facility (NERC-ARF) and National Aeronautics and Space Administration (NASA) have been operating for decades (since 1971 in the case of NASA and 1983 in the case of NERC-ARF) and currently still deploy aircraft-mounted hyperspectral sensors for environmental monitoring. These aircraft have been utilised for a wide range of Earth Science related studies including studies on grassland condition such as studies on grassland species diversity in relation to invasive species (Gholizadeh et al., 2019), estimating LAI on grasslands (Atzberger et al., 2015; Punalekar et al. 2018), predicting equivalent water thickness on different vegetation types (e.g. Li et al. 2008) and studies encompassing multiple structural and biochemical grassland variables (Schweiger et al., 2017). Asner et al. (1998, 2000) conducted aircraft RS studies on semi-arid grasslands, shrublands and transition zones (succeeding from grasslands to shrublands) to attribute vegetation variables with the variation of wavelengths in the 400-2500nm spectral region.

### 2.2.3. Satellite remote sensing

Satellite imagery has been used in a wide range of applications which includes vegetation condition monitoring and specifically the monitoring of grassland condition. Some of the earliest remote sensing studies (Jordan, 1969) used vegetation indices derived from satellite data with coarse spatial and spectral resolution relative to satellite data available today. Satellite sensors with a relatively low spatial resolution, such as the Moderate Resolution Imaging Spectroradiometer (MODIS) on the Terra and Aqua satellite platforms, often have the advantage of a relatively high temporal resolution. For example; MODIS collects data with a spatial resolution of 250m-1000m for 36 spectral bands, depending on wavelength, and a revisit rate of 1-2 days) (Maccherone, 2021) and are freely available online. Various studies utilised vegetation indices, where these indices were in some way related to grassland condition, from MODIS satellite products. Wang et al. (2020) and Xu et al. (2013) calculated NDVI from calibrated radiance values for their studies which focused on estimating grassland productivity. Lyu et al. (2020) used Normalized Difference Vegetation Index (NDVI) and Enhanced Vegetation Index (EVI) satellite products provided by NASA to assess grassland degradation in their study, where their methods linked both productivity and ES to grassland degradation. Gao et al. (2006) also focused their study on grassland degradation, but instead used three different NDVI-derived satellite products; MODIS NDVI 10-day product, Advanced Very High Resolution Radiometer (AVHRR) 10-day product and Satellite Pour l'Observation de la Terre (SPOT)-Vegetation 10-day composite NDVI product. Other studies used other satellite products to establish grassland productivity. For example, Zhao et al (2014) used MODIS eight-day net photosynthesis and gross primary productivity (GPP) satellite products in their above ground biomass estimate study.

In contrast, satellites can also have a relatively high spatial resolution at the expense of temporal resolution unless they form part of a large satellite constellation such as Skysat satellites (Planet Labs, 2021). For example, Sentinel-2 is a two constellation satellite system that collects data on the VIS-SWIR parts of the EM spectrum with a spatial resolution of 10-60m (depending on wavelength) and revisit rate of ~5 days whilst Landsat-8 is a one constellation satellite that collects data on the VIS-TIR parts of the EM spectrum with a spatial resolution of 15-100m (also depending on wavelength) and a revisit rate of 16 days. Gu and Wylie (2015) estimated grassland productivity for central Nebraska at a 30m scale using two satellite products; 30-m Landsat 8 Level 1T (terrain-corrected) imagery and the 250m MODIS NDVI product. Xu et al (2014) used Landsat-8 OLI imagery and Landsat-7 Enhanced Thematic Mapper Plus imagery in their study to estimate the dead material component of grasslands in Grasslands National Park, Canada.

It is important that the spatial resolution of satellite imagery is appropriate to the study being conducted. A spatial resolution of 10-300m may be adequate for an effective study of large rangeland areas or homogeneous grasslands, but could be too coarse for studying the condition of fragmented or structurally heterogeneous grasslands (examples of different levels of structural heterogeneity provided in Figure 2.3) (Ali et al., 2016; Dabrowska – Zielinska et al., 2015; Lausch et al., 2016) or for a species-focused RS of grassland condition study (e.g. Wang et al. 2018a). For example, alkaline grasslands that exist within base rich flushes could only be distinguished from surrounding acid grassland by using high spatial resolution imagery as they are less than 10m wide (Smart, S. pers. comm. 12th December 2016). Resolution that is too coarse can lead to irregularities with ground truthing when averaging of *in-situ* data is required during up-scaling (Ali et al., 2016; Dabrowska – Zielinska et al., 2015; Lausch et al., 2016). Alternatively, higher spatial resolution satellite data (such as sub-meter scale imagery from commercial Pleiades satellites) can provide solutions related to low spatial resolution (e.g. Mirik and Ansley) but access to these images can be expensive and will also have a lower temporal resolution (Ali et al., 2016; Chopping et al., 2008). Commercial satellite companies such as Planet Labs seek to overcome the issue of spatial vs. temporal resolution by launching large constellations of relatively small and inexpensive satellites referred to as "microsatellites" or "nanosatellites" (Planet Labs, 2021). It should also be noted that a lack of data collected with other spectral devices within the study area specifically for the purpose of validation may still mean a relatively high amount of error in the results of a RS study (Loew et al., 2017).

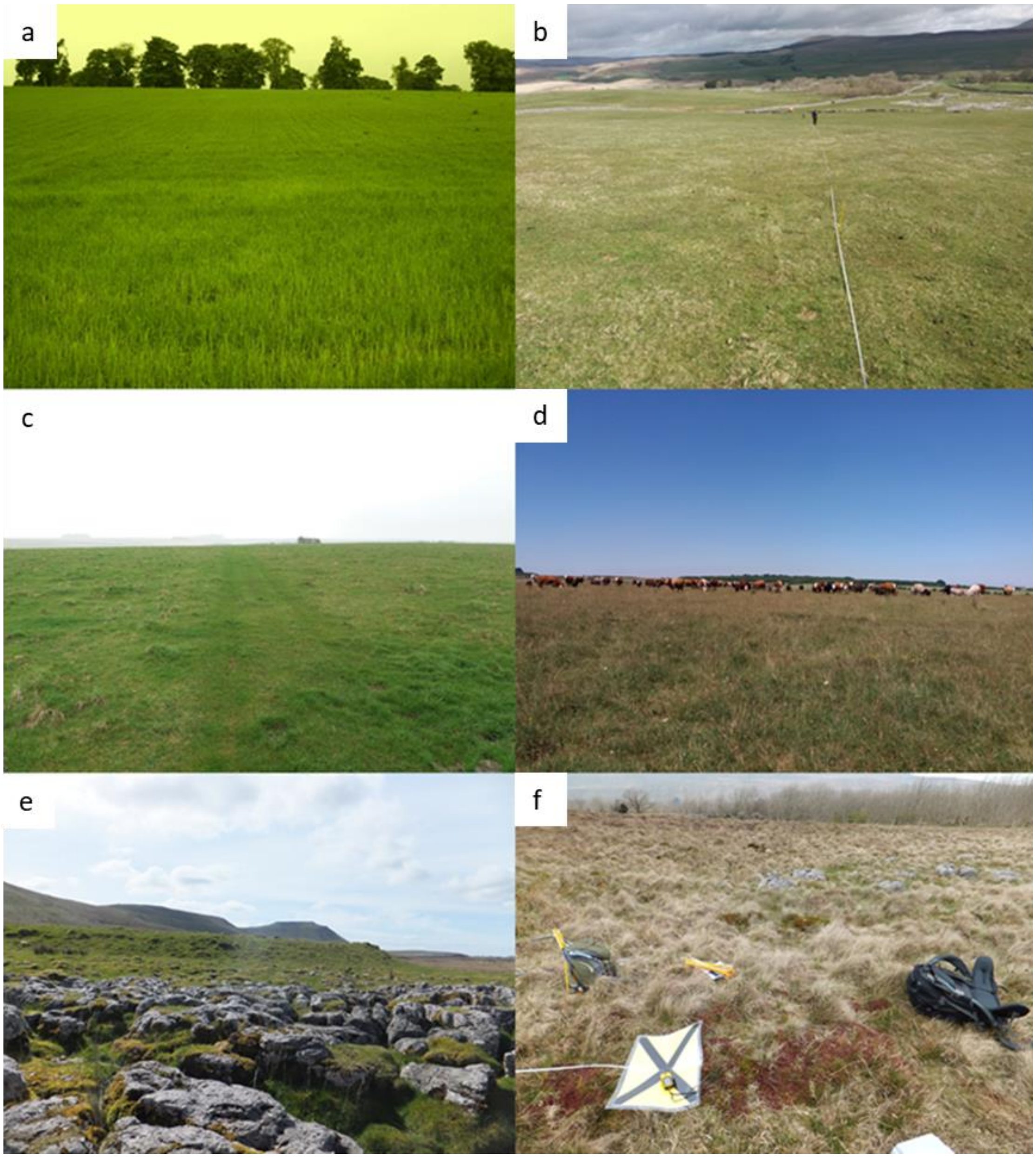



*Figure 2.3: Grasslands representing a gradient of structural heterogeneity from simple to complex: a) monoculture grassland, b) semi-improved grassland (Top Cow Pasture, Ingleborough NNR), c) semi-improved calcareous grassland (100 Acre, Parsonage NNR), d) semi-natural calcareous grassland (Castle Down, Parsonage NNR), e) semi-natural limestone pavement grassland (Scar Close Moss,*

*Ingleborough NNR), f) semi-natural acid mire grassland (Scar Close Moss, Ingleborough NNR).*

# 2.3. Remote sensing approaches for grassland condition-related variables

Many approaches have been taken to monitor grassland condition using remote sensing techniques, targeting a wide range of condition-related variables and using various analytical techniques. A grassland condition study may compare the results of predicting multiple condition-related variables (e.g. Kahmen and Poschlod, 2008; Schweiger et al., 2017) or focus on specific variables (e.g. Pasolli et al., 2015). Some focussed on capturing the process of habitat degradation through land use change (Boyle et al., 2014), others on species diversity or invasive species (Boyle et al., 2014; Lausch et al., 2018), grassland variables such as biomass (e.g. Schweiger et al., 2017) or through the use of at least one of many metrics referred to as spectral traits by Lausch et al. (2018). To predict these variables, the full of spectral range of data collected by at least one spectral device may be used in analysis. Alternatively, specific bands or a combination of bands may be used to predict condition-related variables instead (e.g. Davidson et al., 2006).

Some studies used grassland variables or “spectral traits” to correlate, predict or validate other grassland variables or spectral traits. For example; Wylie et al. (2002) used a combination of destructive samples and spectral data to make modelled estimates of FAPAR as well as LAI and biomass for the North American Great Plains region, then assessed the relationship of these metrics with NDVI. Destructive samples and multispectral data collected with a CROPSCAN MSR 16R were used to derive FAPAR, LAI and biomass, then these metrics were regressed against NDVI which was projected for the region using spectral data from the Landsat Thematic Mapper. Wylie et al. (2002) found that there was a strong correlation between NDVI and all three metrics ($R^2$ >0.9) showing that they have a strong relationship.

The rest of this chapter further explores the wide variety of RS of grassland condition studies that have been conducted so far focussing on the metrics that are most commonly used:

- Biomass, height and % cover
- Leaf area index (LAI), plant area index (PAI) and green area index (GAI)
- Fraction of absorbed photosynthetically active radiation (FAPAR)
- Normalised difference vegetation index (NDVI)
- Specific leaf area (SLA)
- Leaf dry matter content (LDMC)
- Leaf water content (LWC)
- Dead matter and bare ground
- Species richness, indicator species and invasive species
- Biochemical variables

*Table 2.2: Specifies the number of papers discussed in Section 2.3 (with total number of references for each section in parentheses) and also some characteristics of those papers, such as which RS platforms were used and whether the metric in question was used as a predictor or response in models. Note that multiple spectral devices are often used in RS studies, in particular data from at least one hand-held device and at least one non-terrestrial device (UAV, aircraft or satellite). Also note that some studies used a metric as a response variable and as a predictor of other metrics.*

| Metrics | Number of references | Hand-held | UAS | Crewed aircraft | Satellite | Predictor | Response |
|---|---|---|---|---|---|---|---|
| Biomass, height and % cover | 5 (17) | 3 | 1 | 0 | 4 | 0 | 5 |
| LAI, PAI and GAI | 6 (22) | 5 | 0 | 1 | 4 | 0 | 5 |
| FAPAR | 4 (6) | 3 | 0 | 0 | 2 | 0 | 3 |
| NDVI | 6 (12) | 1 | 0 | 0 | 6 | 6 | 0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| SLA | 3 (12) | 2 | 0 | 0 | 1 | 3 | 0 |
| LDMC | 3 (10) | 1 | 2 | 1 | 1 | 0 | 3 |
| LWC | 3 (3) | 2 | 0 | 0 | 2 | 0 | 3 |
| Dead matter and bare ground | 3 (14) | 2 | 0 | 0 | 3 | 0 | 3 |
| Species richness, indicator species and invasive species | 5 (10) | 2 | 1 | 3 | 1 | 1 | 4 |
| Biochemical variables | 4 (9) | 4 | 2 | 1 | 0 | 0 | 4 |

### 2.3.1. Biomass, height and % vegetation cover

Many studies have focused on or incorporated biomass, grass height and/or other productivity measures into their study to establish grassland condition with respect to ecosystem services (e.g. Homolová et al., 2014) or grassland productivity (Bullock et al., 2011; Schils et al., 2013) and have used one of these grassland variables to help determine another. For example, productivity can be determined by weighing destructive samples taken from a defined area which is then combined with grass height measurements to derive biomass (Bai et al., 2001; Psomas et al., 2011). Alternatively, the mass of destructive samples from a defined area alone is used (e.g. Schweiger et al., 2017).

Changes in biomass can be related to the degradation of grassland condition and associated socio-economic and ecological impacts (Gao et al., 2006; JNCC, 2004; Lyu et al., 2020; Psomas et al., 2011). Changes in grassland variables related to biomass such as % vegetation cover and height can also be related to reduced condition. Grass height can be an indicator of degradation (Spagnuolo et al., 2020), undergrazing or overgrazing, all of which negatively impact biodiversity (JNCC, 2004; 2006). The % cover of graminoids and forbs, plus the associated graminoid:forb ratio, are grassland variables that are related to biomass as a greater % cover of these variables means more biomass. Changes in the cover of graminoid species may impact on bryophyte species (Ingerpuu et al., 2005) which are linked to good condition for some grassland types (JNCC, 2004). Few RS studies of grassland condition have separated graminoid from forb biomass, but Schweiger et al. (2017) used PLSR to predict these variables plus a range of other grassland variables using airborne imaging spectroscopy data as predictors. The PLSR models produced $R^2$ results of >0.5 but model performance deteriorated to $R^2$ <0.2 after external validation. Grazing regime (Bai et al., 2001), soil depth, slope and aspect all also have an influence on biomass quantity (Harzé et al., 2016).

Most studies of biomass were conducted at field or regional level; although data collected by satellites or aircraft are often used, an increasing number of studies are conducted using data collected by a UAV. Tucker et al. (1985) used 1km and 4km spatial resolution data from NOAA-6 and NOAA-7 plus ground measurements with a hand-held radiometer and grass clippings to establish the biomass of an area of grassland in the Senegalese Sahel. Zhao et al. (2014) estimated the biomass of the Xilingol grassland using MODIS eight-day PSNnet (net photosynthesis) 1km spatial resolution product and destructive samples collected at 1205 field survey data points for months of July and August for the years 2005-2012. Four different regression analyses, each using a different function, were used to predict biomass using the PSNnet values as predictors and the mass of grass cuttings as a response. All four regression models produced $R^2$ values of 0.55-0.65. Psomas et al. (2011) collected biomass samples and spectral data, using a field spectro-radiometer (i.e. ASD), on grasslands that represented a moisture gradient. These data sets were utilised to predict above-ground biomass at patch level ($1m^2$), then the results were upscaled using either VIs as predictors in ordinary least squares regression or using selected bands used as predictors in multiple linear regression using hyperspectral data collected by the Hyperion EO-1 satellite. The strongest models for predicting biomass at patch level used selected (by branch-and-bound variable searching algorithm) combinations of bands in multiple linear regression which produced $R^2$ values of 0.51-0.86. Marcett et al. (2006) used Landsat 30m spatial resolution imagery (plus ground truthing using a LI-COR LAI-2000 hand-held device) to quantify biomass, height and vegetation cover for managed rangelands in the USA. Vegetation cover was established using the Soil Adjusted Total Vegetation Index (SATVI), plus biomass and height were estimated using a near infrared (NIR) band although the authors believe that a high forb cover (30%) reduced the accuracy of the results. Capolupo et al. (2015) also targeted a wider range of grassland variables when they compared the results of PLSR and multiple vegetation indices (VI) to establish which was best in estimating biochemical and structural grassland variables. UAV-acquired hyperspectral images were collected over two seasons (in May and October) on experimental grassland plots near Kleve, Germany. The results for using VIs as predictors in linear regression models produced $R^2$ results <0.5 for all grassland variables. Using spectral data collected for one season in PLSR produced $R^2$ results =>0.7 for grass height and fresh matter yield. The predictive power of the PLSR models increased when data from two seasons were used in the same model, where the results of predicting most grassland variables were >0.7, with all three structural variables (height, fresh matter yield and dry matter yield) being more strongly predicted with $R^2$ results >0.8.

### 2.3.2. Leaf area index (LAI), plant area index (PAI) and green area index (GAI)

A review by Weiss et al. (2004) has covered how LAI is defined, the theoretical background behind the RS approach to measuring LAI and the reasons for using LAI in a grassland condition study. Shen et al. (2014) covers a range of methods and also reasons for measuring LAI. Because of the extensive information provided in these reviews, only a summary of LAI is provided in this thesis. The way that leaf area index (LAI) is defined, measured and and/or calculated has changed over time. LAI is traditionally defined as leaf area density over canopy height but can also be defined as half the total developed area of leaves per unit ground horizontal surface area (Weiss et al., 2004). LAI is a common choice for grassland condition RS studies because LAI (plus leaf angle distribution and leaf water content) is considered to be one of the dominant controls on canopy reflectance data for dense canopies (Asner, 1998; Roelofsen et al., 2015).

LAI is related to canopy biomass, grassland density, stress (in the context of LAI, this refers to increased bare ground), growth or productivity, grassland structural heterogeneity (a proxy for biodiversity), management practices (Dusseux et al., 2014; Haboudane et al., 2004; He et al., 2007; Möckel et al., 2014; Yang and Guo, 2014; Zhang et al., 2020) and water content (Davidson et al., 2006; Sibanda et al., 2019). Because of this, other important calculations linked to grassland condition can be derived from LAI. For example, Anderson et al. (2004) stated that there is a linear relationship between LAI and vegetation water content and Davidson et al. (2006) utilised LAI when calculating canopy level equivalent water thickness (EWT).

*In situ* approaches of capturing LAI during data collection are summarised by Weiss et al. (2004) and a range of traditional and RS methods of data collection are discussed by Shen et al. (2014). Destructive methods for measuring LAI, such as the conveyor belt method (where LAI is derived by scanning individual leaves placed on a conveyor belt), is time-consuming which results in small sample sizes (Roelofsen et al., 2014). This has encouraged the use of RS techniques to measure LAI (Shen et al. 2014; Weiss et al., 2004).

Remote-sensing grassland condition studies have used hand-held devices and/or satellite data to estimate LAI (Shen et al. 2014) and have also renamed and/or redefined LAI as plant area index (PAI) (Asner et al., 2000) or green area index (GAI) (Pasolli et al., 2015). When collecting RS data on the ground using handheld devices, many studies used a LAI-2000 (LICOR, Lincoln, NE) Plant Canopy Analyser to estimate LAI or PAI (Haboudane et al., 2004; He et al., 2007; He and Guo, 2006). Grassland LAI studies have also measured GAI of alpine grasslands using a Li-3100 portable leaf area meter (Pasolli et al., 2015) and measured grassland LAI using a combination of destructive sampling and an AT leaf area meter (Curran and Williamson, 1987).

Many studies that used LAI also utilised satellite products to conduct large-scale studies, where destructive samples and/or RS data collected at ground level were used for ground-truthing. Pasolli et al. (2015) estimated LAI using Moderate Resolution Imaging Spectroradiometer (MODIS) satellite imagery (with ground truth data from a Li-3100 LICOR hand-held device) for mountain grasslands in the Alps. The accuracy of these measurements (RMSE accuracy of 1.68 $m^2$) was considered by the authors to be an improvement on previous studies in such difficult terrain, this improvement was attributed to customised MODIS data and an improved algorithm. He and Guo (2006) used SPOT-4 data and ground measurements using a LICOR

LAI-2000 hand-held device to map the LAI of mixed prairie grasslands in Grasslands National Park, Canada. It was found that adjusted transformed soil-adjusted vegetation index (ATSAVI) was best for estimating LAI for mixed grasslands. ATSAVI was also found to be the best predictor of LAI on semi-arid environments of low vegetation cover by He et al. (2007). Both studies defined ATSAVI as:

$$ATSAVI = \frac{a(\rho_{NIR} - a\rho_{Red} - b)}{a\rho_{NIR} + \rho_{Red} - ab + X(1 + a^2)}, X = 0.08 \qquad (\textit{eq. 2.2})$$

where Red refers to a band within the red part of the spectrum and NIR refers to a band in the NIR part of the spectrum. They have been more broadly defined as different studies choose to utililise different bands within the red and NIR regions of the spectrum. Atzberger et al. (2015) compared four different approaches for estimating grassland LAI; two statistical modelling methods (predictive equations and VIs, referred to as PEre-adjust and vegetation index respectively) and two radiative transfer models (RTM) inversion methods (one based on look-up-tables and one based on predictive equations). Data were collected *in-situ* through destructive sampling and by using a LAI-2000 hand-held device, plus hyperspectral data were collected using the HyMap aircraft. All methods produced $R^2$ values of 0.75-0.91, but it was stated that the accuracy and robustness of the statistical models decreases when fewer samples are used for calibration. Punalekar et al. (2018) combined *in-situ* LAI (collected with a LAI-2000 hand-held device) and field spectro-radiometry (SVC HR 2024i) to calibrate an inverted PROSAIL radiative transfer model to estimate LAI and biomass from 10m Sentinel-2 satellite data on a mixture of pasture and experimental grasslands. Ordinary least squares (OLS) regression produced $R^2$ results between observed and predicted LAI values ranging from 0.61-0.87 across three different grasslands. Schweider et al. (2020) compared the ability of a soil-leaf-canopy radiative transfer model and random forest regression to predict biomass and LAI using Sentinel-2 imagery with field measurements taken using an ASD FieldSpec-2 spectroradiometer hand-held device. Biomass was estimated with a mean $R^2$ of 52% (44-66%) and nRMSE of 17% (14-22%). LAI models performed with a mean $R^2$ of 0.62 (0.44-0.81) and nRMSE of 23% with the two modelling producing similar results.

There are direct and indirect methods of establishing grassland LAI and each has practical issues (Shen et al. 2014). Although non-destructive data collection using a hand-held spectral device is more time-efficient than destructive sampling, it has been shown that there is variability in optical LAI measurements taken on the same samples plus non-destructive sampling underestimates LAI (He et al., 2007; He and Guo, 2006). He et al. (2007) compared the accuracy of two different hand-held instruments (LAI 2000 and AccuPAR) with destructive sampling for estimating LAI. He et al. (2007) showed that the lower the LAI of four grassland communities studied, the greater the underestimated percentage of LAI values collected using RS devices relative to destructive sampling.

He et al. (2007) suggested that this underestimation was due to three reasons. Firstly, placing a sensor onto grass disturbs it resulting in higher incident light deeper in the canopy and therefore an underestimation of leaf interception and LAI. Secondly, the instruments calculate LAI using absorbed radiation to establish the amount of light intercepted by the canopy, ignoring leaf transmission scattering and all second-order radiative effects in three-dimensional space. The aforementioned issues are referred to as radiative error and are believed to contribute to an underestimation of LAI. Lastly, the measurements are calculated based on an assumption that there is a random distribution of foliage which may not be true of some grassland patches.

This underestimation appears to be inconsistent in the literature and therefore cannot be corrected to match destructive sampling. Furthermore, it would not be practical to use a RS technique to collect data on heavily grazed grasslands which have blades that are shorter than the instrument height (Gerard, F. pers. comm. 12th June 2017). This explains why LAI estimation studies have been carried out on croplands (Bacour et al., 2002; Haboudane et al., 2004), prairies (He et al., 2007; He and Guo, 2006) and woodlands (e.g. Chen et al., 1997) which have relatively tall vegetation.

### 2.3.3. Fraction of absorbed photosynthetically active radiation (FAPAR)

The fraction of absorbed photosynthetically active radiation (FAPAR) refers to the absorbed fraction of the photosynthetically active radiation (PAR) part of the EM spectrum (considered to be within the 400-700nm range) (Asner et al. 1998). Spectral data can be used to calculate FAPAR, but satellite products such as the MODIS LAI/FPAR product can be downloaded with this metric already calculated for the user. Aside from being used as a metric in estimating variables related to vegetation condition such as net primary productivity and greenness, FAPAR is also used as a parameter in climatological (because it is associated with the carbon cycle) and ecological models (Tao et al. 2016).

Olofsson and Eklundh (2007) exploited the relationship between FAPAR and NDVI by using NDVI to model FAPAR for various sites in the Scandinavian region which had a mixed cover of trees, shrubs and grass species. NDVI came from MODIS satellite data and the modelled FAPAR was validated against ground measurements. For all sites, the RMSE of mean (%) ranged from 0.33% to 31% with an average of 6.9%. Rossini et al. (2014) used a range of VIs and PAR as variables in their models to derive gross primary productivity (GPP) on sub-alpine grasslands. The models had relative root mean square deviation (rRMSD %) values ranging from just under 20% to over 50%. Schile et al. (2013) estimated the FAPAR on Californian wetlands with a high % cover of dead material, where FAPAR was used as a proxy for productivity. A range of unspecified VIs were calculated using data collected at different depths of the vegetation with a ASD FieldSpec Pro and used as independent variables in pairwise correlation of FAPAR. The dependent variable (FAPAR) was calculated from incoming and transmitted photosynthetically active radiation measurements taken in the field at three different levels (heights) of the vegetation. The findings suggested that a high % dead material cover had a negative impact on the strength of correlation between VIs and FAPAR, plus the structure of wetlands (in particular the very tall vegetation relative to other grassland types) make capturing grassland variable data difficult. Another drawback to using FAPAR as a condition metric is that FAPAR satellite products have low spatial resolution (300m or 1km). Some studies overcame this by calculating FAPAR themselves using higher spatial resolution satellite imagery.

### 2.3.4. Normalised difference vegetation index (NDVI)

Normalised difference vegetation index (NDVI) is a measure of the difference between two spectral bands collected on a given space, one wavelength from the red region of the spectrum and another from the NIR region (Tucker, 1979). Exactly which wavelengths are chosen, and how wide the bandwidths are, depends on the spectral device used for data collection. NDVI can be calculated as:

$$(\mathrm{NIR} - \mathrm{RED}) \,/\, (\mathrm{NIR} + \mathrm{RED}) \qquad (eq.\ 2.1)$$

NDVI is considered to be related to grassland condition as NDVI has been linked to LAI, biomass, FAPAR and GPP which are used as proxies of condition (Chapungu et al., 2020; Chen et al., 2009; Corbane et al., 2013; Gu and Wylie, 2015; Wang et al., 2020). This link has been utilised in land use classification studies (Corbane et al., 2013; Geerken et al., 2005) and cutting/grazing regime studies (Halabuk et al., 2015). NDVI is almost always calculated at regional scale using satellite products for vegetation condition monitoring. Satellite products came from a range of satellites, but the most common satellite product for most of the studies that focused on using NDVI and on grassland condition utilised Moderate Resolution Imaging Spectroradiometer (MODIS) satellite imagery or the vegetation index 16-day global NDVI product derived from MODIS imagery (e.g. Halabuk et al., 2015; Xu et al., 2013).

Many studies that used NDVI as a grassland condition-related metric utilised satellite products to conduct large-scale studies. Xu et al. (2013) calculated NDVI from MODIS imagery acquired during the May-September period for the years 2003-2008 to use as a proxy to map productivity for all grasslands in China, broken down by region. Productivity was used as a proxy for grassland condition, where relatively higher productivity was considered to demonstrate good condition. Gu and Wylie (2015) also used a MODIS NDVI satellite product (250-m MODIS GSN where GSN refers to growing season NDVI) where NDVI was used as a proxy to map productivity, but this time for Nebraska (USA). Gu and Wylie (2015) then used 30-m Landsat Thematic Mapper (TM) data to downscale their productivity map. Piecewise regression showed a strong correlation between predicted GSN and actual GSN (r = 0.97, average error = 0.026). On the other hand, some studies found that NDVI was a weak predictor of biomass. Chen et al. (2009) attempted to estimate biomass on alpine meadows in China by using a range of narrowband VIs (including NDVI) as predictors in a PLSR model. The strongest PLSR model ($R^2$ = 0.27) was produced by using NDVI calculated using 746nm and 755nm wavelengths. Psomas et al. (2011) tested the ability of a range of VIs (including NDVI) and selected bands to predict biomass at patch level ($1m^2$) using ASD data (unlike the previous three studies discussed in this section which did not use any ground truthing), before upscaling the results. Although the patch level results, using four variants of NDVI, produced $R^2$ values 0.51-0.65, using selected combinations of individual bands in multiple linear regressions produced higher $R^2$ values of 0.51-0.86.

Using NDVI is particularly disadvantageous when calculated on grasslands with a relatively high % cover of litter. Xu et al. (2014) explored the relationship between NDVI and dead material cover to investigate how changes in dead material alter the relationship of total biomass and NDVI using destructive samples and Landsat imagery. Positive/negative relationships between total biomass and NDVI only existed where dead material consisted of <20% or >80% of total cover. Guo et al. (2005) showed how dead litter complicates analyses (e.g. using VIs as predictors in models) not designed for heterogeneous landscapes such as mixed prairie grasslands. It was found that NDVI is not suitable for biomass estimation whilst leaf area index (LAI) had stronger results although LAI could only explain 59.8% variation of total biomass. LAI was able to explain 81.5% of variation of plant moisture content (absolute difference between wet and dry biomass in this case) compared to 53.2% for NDVI. The study site included grazed and non-grazed sites, but the percentage of dead material and exact nature of grazing was not specified.

### 2.3.5. Specific leaf area (SLA)

Specific leaf area (SLA) is the one-sided area of a fresh leaf divided by its dry mass, where the lamina (leaf blade) is used for area measurements of grass samples which are usually oven-dried at 60-80$^{o}$c for 48-72 hours (e.g. Molinari and D’Antonio, 2014) then weighed to ascertain dry mass. SLA has been used in previous traditional and RS of grassland condition studies as a lower SLA can be an indicator of reduced grass moisture or nutrients (Harzé et al., 2016, Liu et al. 2017) and can also be used to calculate other metrics related to grassland condition (Ferreira et al., 2011; He et al., 2007). For example, He et al. (2007) calculated LAI from SLA and Ferreira et al. (2011) used SLA and biomass values derived from destructive sampling to establish equivalent water thickness (EWT). Liu et al. (2017) calculated SLA for four dominant grassland genera in Northern China. They also linked SLA to condition-related variables such as nitrogen content and also related soil and climatic variables such as soil nutrient content, mean annual precipitation and mean annual temperature.

One disadvantage of this approach is that data collection can be time-consuming as the leaf area of individual grass blades has to be measured using leaf area measuring software or a ruler (e.g. Harzé et al., 2016) meaning that either proxies are used or only a small sample set is collected (e.g. Roelofsen et al., 2014; Wellstein et al. 2017). Proxies and databases have been used to represent SLA in some studies (e.g. Möckel et al., 2014) to avoid time-consuming data collection. Furthermore, some studies suggest that the variability of SLA within each grassland and between different grasslands is relatively high compared to some other spectral traits (Firn et al., 2019; Harzé et al., 2016).

Another disadvantage is that other variables are more effective and practical for establishing grassland condition than SLA. Roelofsen et al. (2014) found that specific leaf area and nutrient-related variables (N and P content) was poorly predicted from any spectral data whilst leaf dry matter content was more strongly correlated with spectral data. Smart et al. (2017) found that Leaf Dry Matter Content (LDMC) predicted above-ground net primary productivity (aNPP) better than SLA and could be measured *in situ* in a more time-effective manner. Pakeman et al. (2011) tested whether LDMC, SLA or three biochemical variables (C, N and C:N) could be used to train a linear regression or exponential model to predict grassland litter decomposition. It was found that LDMC was the best predictor, although models trained using LDMC still had weak predictive power (best result of $R^2$ = 0.334).

### 2.3.6. Leaf dry matter content (LDMC)

Leaf dry matter content (LDMC) is defined as the ratio of leaf dry mass to fresh mass (Garnier et al., 2001) and like SLA, is related to productivity (Ali et al., 2019; Smart et al., 2017). LDMC can be calculated by weighing vegetation leaves acquired from destructive sampling before and after oven-drying (Garnier et al. 2001). LDMC has been linked to other condition-related grassland variables such as biomass (Polley et al. 2020) and nitrogen content (Polley et al. 2022) and also linked to vegetation indices such as NDVI (Polley et al. 2020). Studies that used LDMC as a condition metric were conducted at a range of scales and using a wide range of spectral devices, but most studies were conducted at field or regional scale and utilised satellite products.

Roelofsen et al. (2014) collected spectral data on individual leaves in a laboratory (400-1800nm spectral range of 35 species) and tested the strength of correlation between these spectral data and a range of structural and biochemical variables. LDMC had higher $r^2$ values (0.57-0.58) than other morphological and biochemical variables which had correlation values $r^2$ <0.3 except leaf nitrogen content (0.46-0.66). Ali et al. (2019) compared the performance of PLSR and 11 different VIs to predict LDMC on wetlands in the Netherlands where Sentinel-2 spectral data were used as predictors. Using spectral data in PLSR produced the strongest prediction of LDMC ($R^2$ = 0.71) although four of the eleven VIs produced relatively strong results in predicting LDMC ($R^2$ = 0.67). Polley et al. (2020) used patch level spectral data collected by a drone on both semi-natural and monoculture grasslands in PLSR models to predict LDMC at both leaf level and canopy level. The results of these models were then extrapolated to field level using spectral data collected from an aircraft. The PLSR models were reported to explain 62% and 73% of the variance in LDMC of individual leaves and canopies respectively. It is assumed that these results are at patch level, it is not made clear how well these models perform when extrapolated to field level using airborne collected spectral data. It was also found by using variable importance in projection (VIP) that the red edge and NIR spectral bands were the strongest predictors of LDMC. Polley et al. (2022) also used patch level spectral data on semi-natural and monoculture grasslands, this time collected using a drone and ASD hand-held spectrometer, to predict LDMC using PLSR with a $R^2$ value of 0.73. Roelofsen et al. (2014) tested the strength of correlation between the spectral signature of individual leaves (400-1800nm spectral range of 35 species) measured in a laboratory and a range of structural and biochemical variables. LDMC had higher $r^2$ values (0.57-0.58) than other morphological and biochemical variables which had correlation values $r^2$ <0.3 except leaf nitrogen content (0.46-0.66).

There are advantages to using LDMC over SLA, for example LDMC correlates more closely with spectral data than SLA (Roelofsen et al., 2014). Furthermore, it is easier to take ground measurements of LDMC and it is a more effective proxy than SLA for grassland variables such as net primary productivity and litter decomposition (Pakeman et al., 2011; Smart et al., 2017). LDMC has the disadvantage of being time-consuming to measure (as measurements of individual blades of grass are being taken) resulting in a low sample size (Shipley and Vu, 2002) and has high within-grassland variability (Harzé et al., 2016).

### 2.3.7. Leaf water content (LWC)

Moisture content is defined as the difference in weight (gram or % for absolute or relative moisture content respectively) between wet grass sample mass and dry grass sample mass and is linked to drought and wildfire risk. Like SLA and LDMC, measuring LWC requires oven-drying grass cuttings which are weighed before and after oven-drying (Davidson et al., 2006). Davidson et al. (2006) applied VIs, “band combinations” and “derivative combinations” with OLS regression to predict absolute and relative vegetation water content (AWC and RWC respectively) on a prairie grassland–shrubland at patch level using CROPSCAN hand-held spectrometer data. “Band combinations” and “derivative combinations” were combinations of bands that were potentially the best predictors based on a modified bootstrap approach but these bands were not specified by the authors. The results of predicting AWC and RWC were then upscaled from patch level (0.5m spatial resolution) to field level (30m spatial resolution) to make the spatial resolution comparable to Landsat TM imagery. It was found that “band combinations” predicted AWC with high $R^2$ and RMSEP values ($R^2$ = 0.8 and RMSEP = 48.4 at patch level and $R^2$ = 0.73 and RMSEP = 53.1 at field level) as did some VIs ($R^2$ = 0.76 and RMSEP = 51.7 at patch level and $R^2$ = 0.7-0.71 and RMSEP = 52.6 at field level). RWC predictions were less accurate, but once again using band combinations performed best with results of $R^2$ = 0.53 and RMSEP = 0.05. Li et al. (2008) used leaf-level data and NASA AVIRIS aircraft spectral data to estimate equivalent water thickness (EWT). At leaf level, EWT was estimated with $R^2$ values during calibration and validation >0.99. When modelling with data from AVIRIS, the $R^2$ values were $R^2$ = 0.87 after calibration and $R^2$ = 0.78 after validation. Ferreira et al. (2011) quantified the spatial and temporal variability of vegetation (forest, shrubland and grassland) water content in the Cerrado of Brazil using EWT. EWT was derived from ground-based measurements of SLA and leaf water concentration. EWT was predicted at patch level and then up-scaled using two different approaches, one approach used an unspecified regression analysis (possibly OLS regression) and Earth Observing-1 (EO-1) Hyperion satellite imagery. The other approach applied a different unspecified regression analysis (also possibly OLS regression) to the MODIS vegetation index 16-day 250m spatial resolution global product. The outcome of extrapolating the results using these two different satellite products were compared and the lower spatial resolution (250m) MODIS product appeared to give lower canopy EWT values relative to the EO-1 Hyperion satellite 30m spatial resolution imagery. As part of a wider study conducted on experimental grasslands, Sibanda et al. (2019) used spectral data collected using an

ASD FieldSpec Pro plus data from two hyperspectral satellites (HyspIRI and EnMAP) to train PLSR and sparse PLSR models to estimate EWT. Models were trained on each of the twelve experimental grasslands that represented a range of different fertiliser treatments, and also trained on either HyspIRI or EnMAP data. The results presented in the figures of the paper are from trained sparse PLSR models as these apparently outperformed PLSR models. The $R^2$ values from models trained with HyspIRI data seemed to range from approximately 0.5-0.9 whilst models trained with EnMAP data ranged from approximately 0.2-0.7. Wavelengths close to the water absorption bands in the upper NIR and SWIR regions of the EM spectrum were the strongest predictors of EWT.

## 2.3.8. Dead matter and % bare ground cover

Dead material, in the context of this thesis, refers to any above-ground necromass belonging to a floral species whilst bare ground refers to any non-vegetated surface including bare soil and rock. Dead material can consist of standing senesced plants or overlying litter (Xu et al., 2014; Yang and Guo, 2014). Dead material is used as an indicator of disturbance level (Xu et al., 2014) or management intensity as this variable is influenced by grazing regime, cutting and fire (Franke et al., 2012; Xu et al., 2014). For example, a build-up of litter can be the result of a lack of hay collection or undergrazing which can affect species composition (JNCC, 2004; 2006). Particular species produce relatively large amounts of litter, and the species in question may be a positive or negative indicator species depending on the grassland type (Gerard et al., 2015).

Studies (e.g. Möckel et al. 2014) have linked an increased % cover of bare soil with a reduction in grassland condition. Common Standards Monitoring (CSM) guidance recommends bare soil cover of <5% for most grassland types although a relatively higher (unspecified) % cover of bare soil is accepted for certain acid and calcareous grasslands. A low percentage of bare soil is seen as more beneficial than no bare soil as it promotes the regeneration of grass from seed, but a relatively high % cover of bare soil may also be considered unfavourable as undesirable species (such as invasive or highly competitive species) are more likely to colonise the bare patch (JNCC, 2004). Möckel et al. (2014) tried to classify different successional phases on grasslands and used bare soil as an indicator of condition. Their study assumed gradual degradation (as increased % bare soil cover) for all fields with time plus dead litter was removed during data collection.

Guo et al. (2005) investigated the relationship between spectral data and *in situ* grassland measurements on a range of grassland variables in a native mixed prairie ecosystem, which included study sites that had a relatively high litter content. Data were collected using two hand-held devices (to collect hyperspectral data and LAI measurements) on a total of sixty 100m transects. Correlation analysis was run between biophysical variables and NDVI then LAI respectively with the Jack-knife used as a validation technique. Regression analysis was used to predict total biomass and plant moisture content from NDVI and LAI separately. All biophysical variables except moisture content ($r = 0.729$) had low r values when using NDVI in analysis. Using LAI produced r values >0.7 for graminoids, dead material and moisture content. Xu et al. (2014) calculated a range of indices using Landsat 7 imagery to test their potential as predictors to estimate dead cover. The results suggest that the dead component can be estimated with multispectral images using Normalized Burn Ratio (NBR) or Normalized Difference Water Index (NDWI), but the relationships are highly influenced by bare soil and soil crust, i.e. are only significant when bare soil and soil crust are <20% of cover.

It has been stated in a number of papers that dead material and bare soil complicate RS studies of heterogeneous grasslands (Asner, 1998; Asner et al., 2000; He and Guo, 2006; Schile et al., 2013; Shen et al., 2014; Xu et al., 2014; Yang and Guo, 2014; Zhao et al., 2014). Xu et al. (2014) partly attributed this complication to a similarity in spectral signature between dead litter, bare soil and soil crust (i.e. bryophytes), with the only main difference in part of the shortwave infrared region (~2000 nm). Xu et al. (2014) and Yang and Guo (2014) show how different ratios of bare soil, dead material and green grass within a study site change the shape of the grassland spectral signature in specific places and in a subtle way. Dead material also causes an increase in variation of the spectral signature on the same grassland type (Asner et al., 2000; Xu et al., 2014). Furthermore, it was stated by Asner et al. (2000) that the presence of dead material could be detected in the spectral signature, but not quantified.

### 2.3.9. Species richness, indicator species and invasive species

Species richness is the absolute number of species within a defined space, which is not to be confused with species abundance which refers to the relative abundance (usually captured as % cover) of each species within a defined space. Positive indicator species are species considered to be indicative of a particular grassland community with negative indicator species being their antithesis. Invasive species are described as non-native species that have a negative impact on their new environment, where this negative impact could refer to reduced biodiversity for example (JNCC, 2004; 2006).

Several studies have associated particular grassland species or communities with condition as part of a specific grassland variable study (e.g. Bai et al. (2001) focused on biomass), as a proxy for other condition-related variables (e.g. Roelofsen et al., 2015), part of a more holistic study (e.g. Homolová et al., 2014) or wider framework to label a particular grassland by type or condition (e.g. JNCC, 2004). These studies were conducted at a range of scales, with studies utilising spectral data collected from a UAV becoming increasingly common.

Wang et al. (2018) used data from multiple ground-level spectral devices and the aircraft-mounted AISA Eagle imaging spectrometer to link spectral variation with grassland biodiversity in Minnesota, USA. Zaman et al. (2011) used multispectral imagery from a UAV to identify the spread of an invasive species (*Phragmites australis*) in wetlands in Utah, USA. Roelofsen et al. (2015) used indicator species as part of a remote sensing study to indicate soil pH and groundwater levels. Schweiger et al. (2017) reiterated that indicator species are related to soil biogeochemistry plus biochemical and structural grassland variables. Möckel et al. (2014) used indicator species as part of a RS study to identify grasslands at different levels of “succession” which actually related to management type and degradation. Mansour et al. (2016) mapped grassland degradation using SPOT 5 data by using the distribution of indicator species as a proxy for degradation. Edaphic factors derived from soil samples (including soil chemistry) were used to improve the classification accuracy, including edaphic (soil-related) factors was reported to have increased the classification accuracy by 13% to 88.60%.

Noss (1990) summarised the ideal indicator species but also stated that one limitation to this approach is that it is possible that the indicator species may not indicate anything about some environmental trends. Xu and Guo (2015) stated that many variables are not taken into consideration when only using indicator species in a study such as energy flux, nutrient cycle, productivity, diversity or response capacity to disturbance. This is possibly because data collection for species richness or abundance is also time-consuming, limiting time to collect data on other variables (JNCC, 2004). Despite this, the use of indicator species as part of a more comprehensive study was still recommended by Noss (1990).

### 2.3.10. Biochemical variables

There are a wide range of biochemical grassland variables used as proxies of grassland condition in the literature such as chlorophyll, nitrogen and phosphorus which are linked to plant stress (i.e. nutrient deficiency) (Lausch et al., 2018). Estimating canopy biochemical variables from remote sensing is usually carried out using hyper-spectral reflectance signatures where particular bands or regions of the spectral signature are sensitive to changes in a particular chemical, for example the chlorophyll absorption peaks within the visible region of the EM spectrum. Destructive grass samples are analysed in a laboratory to ascertain the concentration of chemicals targeted by a given study (e.g. Asner, 1998). These chemical concentration values are then used as response variables in models where hyper-spectral data are used as predictors.

Many studies have tried to link spectral data and biochemical variables at different scales but most of these studies focus on forests (e.g. Asner et al., 2011; 2015) with few studies being conducted on grasslands. Polley et al. (2022) used patch level spectral data from a drone and ASD hand-held spectrometer to predict community nitrogen levels with a $R^2$ value of 0.87 using PLSR. Wang et al. (2019) compared the ability of PLSR and Gaussian processes regression to predict fifteen different grassland biochemical and structural variables on experimental grasslands using data from the NASA AVIRIS aircraft. Both modelling approaches predicted all variables except lignin and chlorophyll a + b with $R^2$ values > 0.55 (some with $R^2$ values > 0.8). The biochemical variables predicted by models with a moderate to strong predicting power included nitrogen, carbon, carbon:nitrogen ratio, hemicellulose and cellulose. Capolupo et al. (2015) compared the results of PLSR and multiple vegetation indices (VI) to establish which was best in estimating biochemical and structural grassland variables. Using spectral data collected in a

PLSR model produced $R^2$ results =>0.7 for grass height and fresh matter yield whilst all biochemical variables (except potassium content with $R^2$ results = 0.68) produced $R^2$ results <0.6. Roelofsen et al. (2014) also found that structural variables had a stronger relationship with spectra than biochemical variables in their study on the strength of correlation between leaf-level spectral data and multiple structural and biochemical variables. Apart from leaf nitrogen content (0.46-0.66), LDMC had higher $r^2$ values (0.57-0.58) than all other morphological and biochemical variables which had correlation values $r^2$ <0.3.

A key disadvantage of using biochemical variables in a RS of grassland condition study is the time and cost required to establish chemical concentrations on a sufficient number of destructive samples to effectively train a model. Furthermore, scaling grassland biochemical content from leaf level to canopy level can be affected by confounding variables as grassland canopy reflectance is strongly influenced by vegetation structural properties (He and Mui, 2010). This could explain why structural variables can be more effectively predicted than biochemical variables (Capolupo et al., 2015; Roelofsen et al., 2014).

# 2.4. Summary and conclusions

Lausch et al. (2018) stated that a holistic approach, referring to taking a multitude of environmental and management-related variables into consideration, is required for the effective RS monitoring of grassland condition to capture the non-linear effects of reduced plant condition. This would increase the likelihood of recognising a reduction in condition and acting in a more decisive and targeted way to improve plant condition. Lausch et al. (2018) also accepted that a truly holistic approach, capturing a wide range of inter-related data types, is not practical due to time and resource constraints. This means that conducting a RS of grassland condition study means making difficult decisions on which data sets to collect, including which spectral devices to use and which grassland variables to focus on. This literature review explored which spectral devices, condition-related spectral variables or grassland variables and which framework would be most effective for a RS of grassland condition study. This review also conducted a process of elimination to understand which approaches of the RS of grassland condition are both viable and relatively less explored.

Many RS studies of grassland condition are conducted on experimental grasslands (e.g. Capolupo et al., 2015) or relatively structurally homogeneous grasslands (e.g. Zhao et al., 2014). Many of these studies focused on spectral variables related to the structural or chemical properties of grassland canopies. Some grassland variables, such as dead material (Yang and Guo, 2014) and bryophytes (Cole et al., 2014) have received little attention in previous grassland condition studies and data were only collected over one or two seasons in many of these studies. Very few studies have been conducted in the UK (Cole et al., 2014), none of which utilised multispectral imagery collected by a UAV (e.g. Cupolupo et al., 2015). This is despite the advantages that UAV data collection offers, for example some UK grasslands are fragmented and the use of UAVs in condition studies, rather than satellite products, on fragmented grasslands has been suggested by Dabrowska - Zielinska et al. (2015).

# Chapter 3 – Methods

The primary aim of this research is to assess the link between the definition of grassland condition used in this thesis (CSM-condition, explained in Section 3.4.1) and condition-related grassland variables with grassland spectral reflectance through field and drone spectro-radiometry at a range of spatial-temporal scales. Focussing on semi-natural grasslands within the UK and within the context of ecosystem services (ES), this work addressed the questions specified in Section 1.2 using the methods described in this chapter.

## 3.1. Definition of grasslands and UK grasslands

As grasslands are defined broadly (Reinermann et al., 2020), a definition specific to this thesis is provided in this section. This thesis uses the Dixon et al. (2014) definition of grasslands as a non-wetland type dominated or co-dominated by graminoids and forbs where trees consist of <10% cover and shrubs <25% cover although legumes have also been considered in this thesis in line with some other grassland studies (e.g. Dabrowska - Zielinska et al., 2015). Graminoids consist of the families Poaceae (true grasses), Juncaceae (rushes) and Cyperaceae (sedges) whilst forbs are herbaceous flowering plants that do not include grass families considered to be graminoids. This thesis uses the standard definition of bryophytes, which includes any species considered to be mosses, liverworts or hornworts.

Volume three of British Plant Communities defines different categories of mesotrophic (neutral), calcicolous (alkaline), calcifugous (acid) and montane grasslands according to the National Vegetation Classification (NVC) system. Volume two uses the same system to classify mires and heaths. These subcategories are often divided by a change in species presence and abundance as a result of different treatment but are also related to environmental variables such as surficial geology. An example of this are MG5-MG7 grasslands; where different cutting and/or grazing regimes may have led to a difference in species composition but surficial geology and fertiliser treatment may have also had an effect (Rodwell, 1991; 1992).

# 3.2. Study sites

Halabuk et al. (2015) stated that the success of grassland studies depends mainly on site specific conditions, including the grassland types to be studied. Furthermore, Harzé et al. (2016) conducted a grassland condition study measuring three functional variables (specific leaf area, leaf dry matter content and plant vegetative height) on four calcareous grassland species within three populations. The study showed that for total variability of the considered grassland variables, 0-30% of variance was attributed to between population differences and 70-100% to within population differences. These findings were taken into consideration when choosing the study sites and grassland types. Data were collected on seven temperate semi-natural grassland sites across two locations in England; three grasslands located in the Parsonage Down National Nature Reserve (NNR) and four in the Ingleborough NNR.

Parsonage Down NNR is located in the chalk downs of Salisbury Plain, Wiltshire, UK (51° 10' 42.2159"N, 1° 54' 38.0528"W, Figure 1a). It is a 275-hectare site of special scientific interest (SSSI) and also part of a working farm managed by Natural England. Most of the reserve consists of mixed-grazed calcareous grasslands that represent a range of improvement levels. This location is characterised by chalk geology with associated alkaline soil and calcareous grasslands which are mixed-grazed. Calcareous grasslands are a UK Biodiversity Action Plan (BAP) priority habitat and therefore the monitoring of their condition is mandatory to land managers. Three grasslands were chosen for data collection that represented varying stages of improvement located on the same geology and with the same grazing regime, reducing the possibility of these variables acting as confounding variables (Kahmen and Poschlod, 2008).

Ingleborough NNR is situated in the south-west of the Yorkshire Dales National Park in North Yorkshire, UK (54° 11' 44.5452" N, 2° 21' 0.9432" W, Figure 1b). The reserve covers 1,014 hectares of mountainous karst terrain and contains a range of vegetation types that are associated with (i) a mixed basic and acidic solid geology and drift and (ii) a lowland to upland gradient. The area has calcareous, acid, neutral, improved, semi-improved and reverting grassland plus blanket-bog over gritstone or drift. A variety of grazing regimes exist; sheep, cattle, mixed and no grazing take place on different fields. Data were collected on four grasslands that represent a variety of grassland types and grazing regimes.

Overall, the seven grassland sites were chosen to encompass a range of management styles, grazing regimes, species composition and grassland structural complexity. Maps of each location can be seen in Figures 3.1 and 3.2, a summary of the environmental characteristics of each location is provided in Table 3.1 and a summary of the environmental characteristics of each study site is provided in Table 3.2.

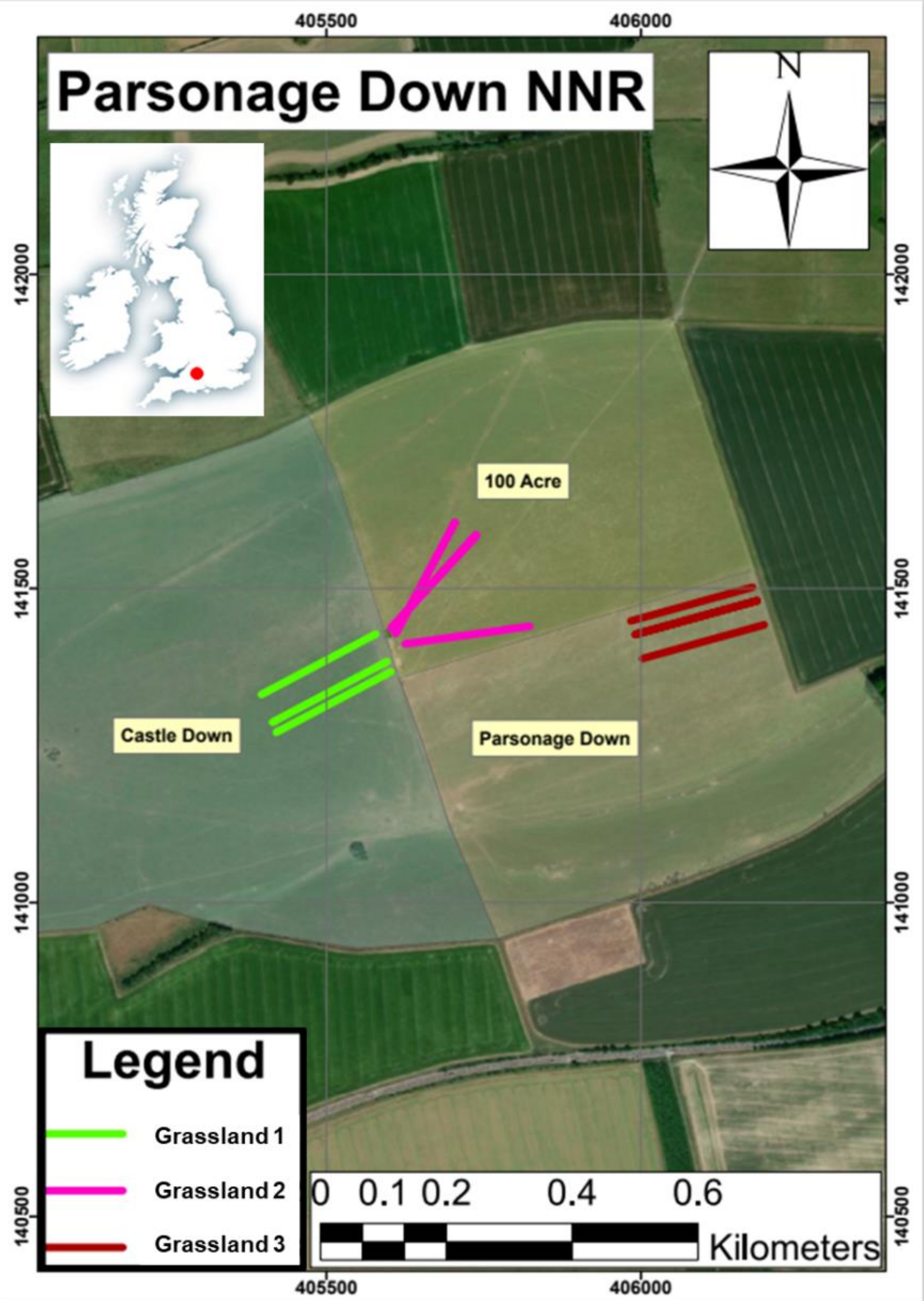



*Figure 3.1 The boundaries and locations of transects 1 to 3 at Parsonage Down NNR. Note that data were collected at this location across three seasons.*

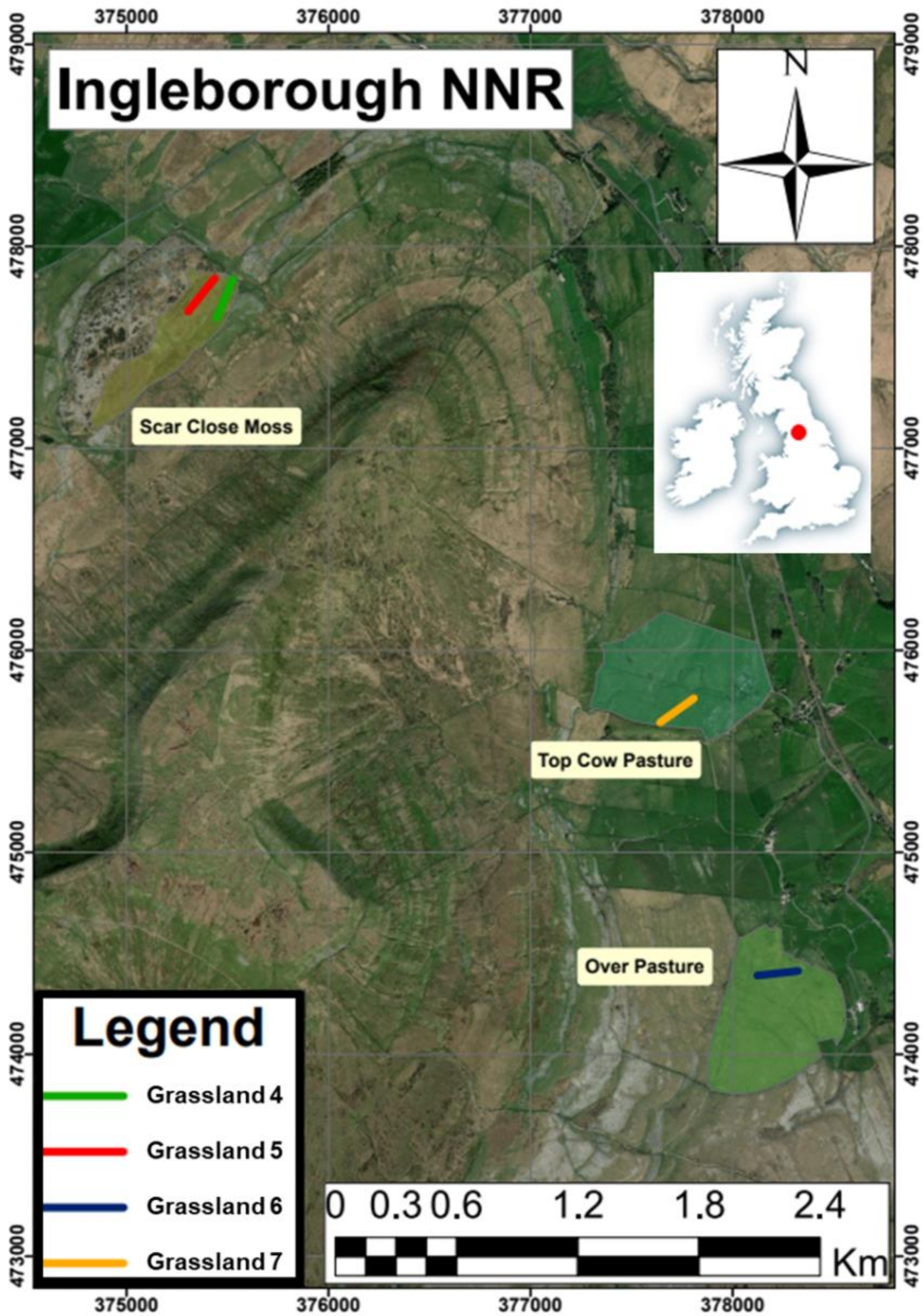



*Figure 3.2: Site boundaries and locations of transects for Grasslands 4 to 7 at Ingleborough NNR.*

*Table 3.1: The environmental characteristics of the two locations chosen for data collection (from information provided by Natural England and by conducting a desk study (BGS UKSO, 2017; Edina®, 2017).*

| **Location** | **Management** | **Geology** | **Soil type** | **Grassland type** |
|---|---|---|---|---|
| Parsonage Down (Wiltshire) | Previously improved mixed grazed grasslands at different levels of reversion | Cretaceous chalk formations (Seaford and Newhaven) | Lime-rich alkaline soil (freely draining) | Chalk grasslands of a range of condition types; improved, reverting, semi-improved and semi-natural |
| Ingleborough (North Yorkshire) | Previously improved, semi-natural, experimental and rewilding grassland plus peat and limestone pavements – sheep, cow and mixed grazing | Danny Bridge Limestone Formation (limestone), Yoredale Group (LST, MST and SST interbeds) plus till | Peat (poor drainage), acidic loamy peaty soils (high drainage) and rendzinas | A variety of types – acid, alkaline, peat bog, limestone pavement |

*Table 3.2: The characteristics of the seven study sites using information provided by Natural England or gained from the desk study (BGS UKSO, 2017; Edina®, 2017). The NVC for each grassland was ascertained by entering species abundance data into MAVIS software (Smart et al., 2016).*

| Site | Site Location | Site Name | Grassland type / NVC | Grazing regime | Improvement level & grazing intensity | Grassland structure |
|---|---|---|---|---|---|---|
| 1 | Parsonage | Castle Down | Chalk grassland / CG2 | Mixed grazing | Unimproved | Relatively long grass with tussocks |
| 2 | Parsonage | 100 Acre | Semi-improved grassland / MG6 | Mixed grazing | Relatively improved | Relatively long grass with tussocks |
| 3 | Parsonage | Parsonage Down | Semi-improved grassland / MG5 | Mixed grazing | Semi-improved | Relatively long grass with tussocks |
| 4 | Ingleborough | Scar Close Moss | Alkaline grassland / CG10 | Sheep grazing | Unimproved but heavily grazed | Closely cropped by grazing, with intermittent limestone pavement |
| 5 | Ingleborough | Scar Close Moss | Acid mire grassland / M19 | Sheep grazing | Unimproved and under-grazed | Relatively long grass with tussocks and heather, plus sinkholes |
| 6 | Ingleborough | Over Pasture | Alkaline grassland / CG10 | Cow grazing | Unimproved | Lightly grazed with a low % cover of limestone |

| | | | | | | |
|---|---|---|---|---|---|---|
| 7 | Ingleborough | Top Cow Pasture | Sloping semi-improved grassland / MG5 | Sheep grazing | Semi-improved and heavily grazed | Closely cropped by grazing, forb dominated in places |

# 3.3. Data collection

The literature review revealed that there were few RS studies using the mass of grassland constituents (e.g. graminoids) as studies that collect destructive samples usually only measure total biomass (such as Schweiger et al., 2017). However, it was thought that collecting and utilising data on mass and % cover would have their own set of advantages and disadvantages. Because bryophytes are sometimes covered by a canopy of graminoids, collecting destructive samples (i.e. mass data) helped establish the amount of bryophytes present, which could have an important impact on reflectance and be missed using the % cover approach. Also, % cover data are compositional data, i.e. relative rather than absolute values, which are constrained to 0-100%. Some analytical methods (e.g. principle component analysis), particularly those using untransformed compositional data and assuming that those data can be projected in Euclidean space, can lead to spurious results as some analyses assume that the data set values are unconstrained and do not transform data as part of the analysis (Gupta et al., 2018; Reimann et al., 2012). Furthermore, there is at least some collinearity in all compositional data because the variables under consideration will always total 100% and an increase in one variable inevitably means a decrease in at least one other variable (Dormann et al. 2012). Using grass cuttings provides the opportunity for establishing biomass, which is often used as a grassland condition measure, plus other grassland constituents can be measured by separating the grass samples into their constituent parts before weighing. On the other hand, establishing mass is far more time consuming than % cover and lacks spatial coverage of the quadrat relative to % cover data.

The grassland variables in Table 3.3 were chosen as it was thought that these variables would be influential to changes in the spectral signature; particularly grass profile (influenced by graminoid:forb ratio), bare soil cover and dead material cover (Asner et al., 2000; Guo et al., 2010; Xu et al., 2014)(Asner et al., 2000; Guo et al., 2010; Xu et al., 2014). Furthermore, it was necessary to collect traditional data on grassland composition to utilise the criteria for measuring grassland condition provided by the CSM documents. Data were not collected on LAI despite this approach being taken by a multitude of RS studies on the basis that LAI is considered to be a dominant control on canopy reflectance (Asner, 1998; Roelofsen et al., 2015) as it was not possible to collect LAI data on very short grasslands (<5cm). It is thought that not taking LAI into consideration is not detrimental to this thesis as biomass, which is considered, is related to LAI (e.g. Möckel et al. 2014). Similar approaches have been used in other RS grassland condition studies where collecting data on LAI was not viable, for example Möckel et al. (2014) used changes in graminoid and bare soil cover as part of a RS of grassland condition study conducted on the island of Öland in Sweden.

*Table 3.3:* Variables *used in this study, listing whether mass and/or % cover data were used to establish them and at which NNR locations they were collected. In the context of this thesis, moisture content refers to leaf wet mass - leaf dry mass).*

| **Grassland variable** | **Type** | **Location** |
|---|---|---|
| Bare ground | % cover | Ingleborough |
| Biomass | mass | Both |
| Bryophytes | % cover, mass | Both |
| Dead material | % cover, mass | Both |
| Forbs | % cover, mass | Both |
| Graminoids | % cover, mass | Both |
| Graminoid:bryophyte ratio (‘gram:bryo ratio’) | % cover, mass | Both |
| Graminoid:forb ratio (‘gram:forb ratio’) | % cover, mass | Both |
| Live material | % cover, mass | Both |

| | | |
|---|---|---|
| Live material:dead material ratio ('live:dead ratio') | % cover, mass | Both |
| Moisture content<br>i.e. *leaf wet mass - leaf dry mass* | % mass | Both |

### 3.3.1. Fieldwork plan and sampling strategy

On each of the seven chosen grasslands, a 200m transect was set up and ten quadrats ($1m^2$) placed along it at random (Figure 3.3) where a random integer generator (https://www.random.org/) was used to choose how far along the transect to place the quadrats. The three Parsonage Down sites were revisited three times during the 2018 growing season (spring, summer and autumn) on the following dates: $16^{th}$ – $20^{th}$ April, $25^{th}$ – $29^{th}$ June and $10^{th}$ – $14^{th}$ September. Radiometers require sufficient irradiance (considered to be 400 $W/m^2$ in this thesis) to operate which eliminates the possibility of data collection during the winter (CROPSCAN Inc., 2018). At the four Ingleborough sites, data were collected during the summer of 2017 ($1^{st}$ – $9^{th}$ July) (see Section 3.6). Each quadrat was geo-referenced using an eTrex 10 GNSS device giving GPS readings with potential spatial accuracies of 2-3m. For sites that were revisited during the growing season, reference points (e.g. fence posts) and photographs were used to relocate quadrats precisely. To locate the quadrats accurately on the drone collected imagery, laminated white A4 sheets (large enough to be visible on the drone imagery) were placed directly opposite the quadrat at a distance of 60cm from bottom-left quadrat corner.

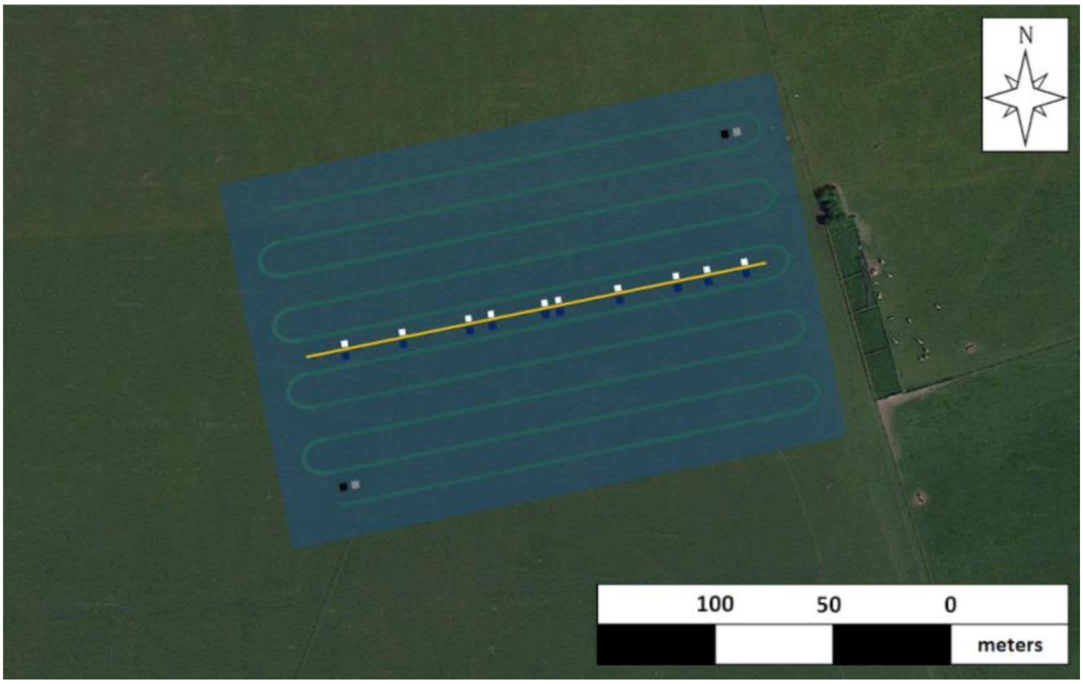



*Figure 3.3: Schematic showing the sampling strategy for data collection (using Castle Down as an example). The yellow line represents the 200m transect and the dark blue squares represent the quadrats. The white squares represent the spatial reference panels and the other grey and black squares represent calibration panels. The green lines are the UAV flight path and the blue rectangle in the background represents the area covered by the UAV-mounted Rikola camera.*

## 3.3.2. Quadrat sampling

On each quadrat, the data was collected using the following sequence: grassland variable % cover estimates, photographs, soil moisture, grass height, species abundance (from which species richness was derived), spectral data and finally destructive samples. For % cover, the grassland variables were: graminoids, forbs, bryophytes, live material, bare ground, dead material and other (see Table 3.3). Percentage cover was estimated by looking straight down onto the quadrat, to the nearest 5%, using the dimensions of the quadrat and a ruler as a spatial reference. Bryophytes were any species that belonged to the bryophyte group of non-vascular plants. Live material cover is the sum total of the % cover of graminoids, forbs, and bryophytes. Bare ground is the % cover of bare soil and rocks. Dead material was considered to be any necromass visible above ground. “Other” refers to something not considered in this study, which was usually dung but also included heather patches on the M19 acid mire grassland. From these variables, two ratios were calculated: graminoid:forb ratio cover and live:dead ratio cover. Quadrat photos were taken with the camera looking straight down. Soil moisture data were collected at five random points on each quadrat using a HH2 Moisture Meter from Delta-T Devices which has a stated accuracy of ± 0.01 $m^3.m^{-3}$ or ±1% and has the functionality to take accurate readings in mineral rich and organic rich soils (Delta-T Devices, 2020). Grassland canopy height was established by taking five randomly located measurements on each quadrat with a ruler. This method was chosen as it is a relatively fast data collection approach and a drop disc compresses grass which would affect the spectral readings (Stewart et al., 2001). Species abundance was established for each quadrat by a botanical expert during spring for Ingleborough NNR and during summer for Parsonage NNR. This thesis defined species abundance as the % cover of each species within a $1m^2$ quadrat, where a botanical expert estimated the cover of each species within each quadrat to the nearest 1% if the cover was 0-5%, or nearest 5% if the cover was >5%. Where % cover exceeded 100%, this was due to more than one layer of vegetation being present. For example, on some grassland types bryophytes were covered by a canopy of graminoids. After all other data were collected including spectral data (see Section 3.3.3), five randomly located $10cm^2$ grass cuttings were taken from each quadrat (see example in Figure 3.4).

*Figure 3.4: An overhead view showing how each quadrat was sampled by destructive sampling.*

The grass cuttings were sorted into the following grass constituents: graminoids, forbs, bryophytes, dead material and other (see Figure 3.5). Long and thin bladed species were considered to be graminoids while broadleaved species were considered to be forbs. Bryophytes were defined as any species that belonged to the bryophyte group of non-vascular plants. Dead material was considered to be any necromass found within a sample. In this thesis, “other” refers to the minute cuts of grass which were too difficult to sort or bits of soil that were accidentally collected. After sorting, grass cuttings were weighed, then oven-dried at $60^{o}$c for 72 hours, and weighed again to determine moisture content (e.g. Bai et al., 2001). As the weighing of grass samples collected in one season took approximately three weeks, the sorted samples would be oven-dried at $60^{o}$c as close to the time of weighing of dry mass as possible to ensure that no moisture was present in the samples. Moisture content was defined as wet mass subtracted from dry mass. Biomass is the sum total of the mass of graminoids, forbs, bryophytes and dead material. Live material mass is the sum total of the mass of graminoids, forbs and bryophytes. Three ratios were calculated: graminoid:forb ratio mass, graminoid:bryophyte ratio mass and live:dead ratio mass. Data on species abundance, grassland height and grassland constituent % cover were used to establish the CSM-condition of each quadrat using the NVC framework (see Section 3.4.1) (JNCC, 2004; 2006).


*Figure 3.5: A grass sample separated into its constituent parts (clockwise from top-left): dead material, graminoids, other, forbs and bryophytes.*

## 3.3.3. Grassland reflectance

### 3.3.3.1. Spectral devices

Before grass cuttings were taken, spectral data were collected using three hand-held radiometers (an Analytical Spectral Device (ASD) FieldSpec Pro, a Spectral Vista Corporation (SVC) HR-1024i and a CROPSCAN MSR 16R) as well as an Uncrewed Aerial Vehicle (UAV) (i.e. DJI Matrice) with a Rikola multispectral camera on board. Table 3.4 lists the spectral characteristics of these devices.

The MSR 16R model of CROPSCAN multispectral radiometer (referred to as CROPSCAN from now on) (Rochester, MN, USA) can accommodate up to 16 bands in the 450-1750 nm spectral range. Upward and downward facing sensors measure both incoming and reflected radiation which is used to calculate % reflectance. To ensure data integrity (George, C. and Gerard, F. pers. comm. 7$^{th}$ July 2016) spectral data was only collected when there was a minimum of 400 watts per metre squared (W/m$^2$) incident irradiance, which is above the recommended minimum of 300 W/m$^2$ (CROPSCAN Inc., 2018). To keep data sets and results comparable, the 16 bands chosen were as closely matching as possible to the bands of the Rikola multi-spectral camera.

The Analytical Spectral Device (ASD) FieldSpec Pro (Analytical Spectral Devices, Boulder, USA, ASD Inc., 2002) and the Spectral Vista Corporation (SVC) HR-1024i field spectrometer (SVC from now on) (Poughkeepsie, NY, USA, SVC, 2012) are very similar hyperspectral instruments which collect data from > 1800 bands that can be interpolated to produce a spectral signature across the 350-2500nm spectrum. Both were loaned by the Field Spectroscopy Facility. The ASD was used to collect data in Ingleborough NNR and the SVC to collect data in Parsonage NNR. This spectro-radiometer collects hyperspectral data in the range of 350-1000nm at 1.4nm intervals plus 1000-2500nm at 2nm intervals (ASD Inc., 2002). Data on 1869 bands are available after water absorption bands have been removed (1350-1460nm and 1790-1960nm).

A drone was deployed to collect multispectral data at the field scale: a custom-built DJI Matrice 600 (DJI, 2018) equipped with a Rikola VNIR camera, referred to as the Rikola camera from now on. This camera has a FOV of 37$^{o}$ and a spectral range of 400-900nm. Thirty bands, each with 10nm bandwidth, can be selected within this range. Like with the CROPSCAN, to keep data sets and results comparable, bands were chosen to be as closely matching as possible to the bands of the CROPSCAN.

Relative to the ASD or SVC, the CROPSCAN collects more limited spectral data but is easier to use in field, making it possible to collect a greater quantity of data spatially. Furthermore, the CROPSCAN has the added convenience of collecting upwelling and downwelling radiation simultaneously. The advantage of using a drone to collect multi- or hyperspectral data over using a hand-held device is that data can be collected on an entire field at a relatively high spatial resolution (6cm using a Rikola VNIR camera). A disadvantage is that data are collected on far fewer bands than some hand-held spectral devices (often only in the VIS and NIR regions of the EM spectrum), such as the ASD FieldSpec Pro, and a smaller region of the EM spectrum relative to many hand-held, aircraft-mounted or satellite-mounted spectral devices due to broad limitations related to the size and weight of the instruments mounted on any <20kg UAV. A more extensive list of the advantages of using UAVs to collect data is given by Anderson and Gaston (2013).

*Table 3.4: Summary of multispectral and hyperspectral devices used in the field.*

| | **ASD FieldSpec Pro** | **CROPSCAN MSR 16R** | **Rikola VNIR camera** | **SVC HR-1024i** |
|---|---|---|---|---|
| **Spectral range** | 350nm–2500nm | 450nm–1750nm | 400-900nm | 350nm–2500nm |
| **Channels** | 2149 | 16 | 30 | 1024 |
| **Bandwidth** *(FWHM*)* | 3nm @ 350–1000nm<br>10nm @ 1000–2500nm | 10nm @ ≤870nm<br>11nm – 1240nm<br>13nm – 1640nm | 10nm | ≤3.3 nm, 700nm<br>≤9.5 nm, 1500nm<br>≤6.5 nm, 2100nm |

| | | | | |
|---|---|---|---|---|
| **Bands chosen** | 1869 bands across 350nm–2500nm – 280 bands in 1350-1460nm and 1790-1960nm ranges removed | 470, 530, 560, 570, 647, 690, 700, 720 740, 760, 780, 850, 850, 860, 870, 1240, 1640 | 515, 530, 531, 550, 560, 570, 647, 655, 665, 675, 687, 690, 700, 710, 720, 730, 740, 750, 760, 770, 780, 800, 810, 820, 830, 840, 850, 860, 870, 880 | 1249 within 350nm–2500nm range - 1024 bands interpolated, then bands in 1350-1460nm and 1790-1960nm ranges removed |
| *** *Full Width Half Maximum*** | | | | |

### 3.3.3.2. Spectral data collection

Using CROPSCAN and either the SVC or ASD spectral data was collected for the randomly placed quadrats along the 200m transect (see 3.3.2). Figure 3.6 shows how each quadrat was sampled using the hand-held spectrometers. To minimise the impact of shading, data were collected two hours either side of solar noon and on hilly sites transects ran up/downhill (rather than across the hill) although this was done as a precaution as the slope of the grasslands in this study was minimal ($<5^{o}$). Quadrats were also kept on the south, west or south-west side of the person collecting the spectral data to prevent the person casting a shadow on the quadrats. Finally, to prevent the tape reflectance contaminating the quadrat reflectance acquired from the drone-mounted Rikola camera, quadrats were placed 60cm away from the tape measure.

The CROPSCAN device was held 2m above the quadrats to collect nadir reflectance from a 1m diameter patch, holding the instrument at 2m was made easy by the design of the device. CROPSCAN data were collected every 1m producing 200 data points. When possible, triplicate data were collected at each data point and then averaged. The raw data were converted into reflectance using CROPSCAN software (processing raw data is explained in Section 3.4.3.1).

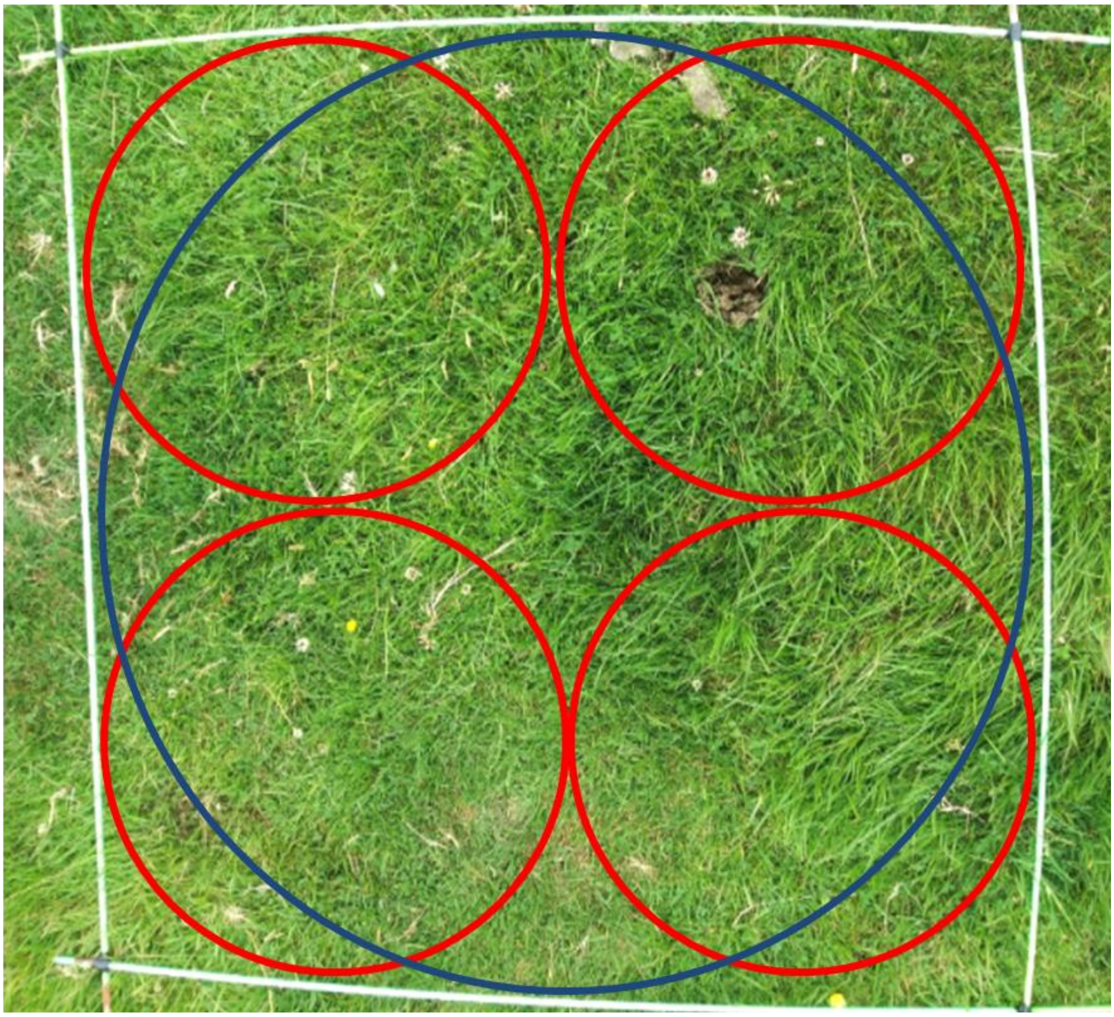


*Figure 3.6: An overhead view showing how each quadrat was sampled using two hand-held spectrometers (blue = CROPSCAN, red = SVC/ASD) and by destructive sampling (black squares).*

Spectral data were collected during the summer season using a SVC at Parsonage Down NNR and an ASD at Ingleborough NNR. The SVC/ASD, fitted with an 18$^{o}$ field of view lens, was held 0.79 m high to take spectral measurements of four 0.25m diameter patches within each quadrat. A tape measure was used to help hold the SVC sensor at 0.79m high. The SVC/ASD collects 25 readings in quick succession, providing the user with one averaged reading. To produce calibrated spectral reflectance signatures (see Section 3.4.3.2) and account for rapid irradiance changes in the field, measurement pairs alternating between the grassland and a white reference panel (Spectralon, Labsphere, NH, USA) were collected. The four patch spectral signatures were averaged into a single quadrat spectral signature. The

Matrice UAV was flown over target fields to cover an area of ~200x200m. White reference sheets were placed along the tape measure near each quadrat so that the quadrats could be located easily in drone images. Grey and black reference images were placed on either end of the study site to help calibrate the Rikola camera.

#### *UAV-mounted Rikola camera*

A UAV with a mounted Rikola VNIR camera was flown across all three grasslands on the 25$^{th}$ June 2018 within two hours of solar noon at a height of ~100m. To ensure the quality of the spectral data being collected, the transects had to be set up to prevent contamination of the spectral signatures of the quadrats by adjacent objects (e.g. by the tape measure) and so that the Rikola VNIR camera could be calibrated. White reference panels were placed adjacent to the quadrats so that the quadrats could be identified in the drone imagery and for the purpose of calibration. Quadrats were placed 60cm away from the A3-sized white reference panels and the tape measure to prevent corruption of the spectral data collected on quadrats. Grey and black reference panels (1m$^2$) were also placed on the outskirts of each field for the purpose of calibrating the Rikola camera. The Rikola camera was calibrated using a black reference panel before flight. Calibrated imagery collected by the UAV-mounted Rikola camera were processed (explained in detail in Section 3.4.3.4) to georeferenced the images, normalise their illumination, calculate the reflectance values for each pixel then finally extract averaged (mean) reflectance values for the 1m$^2$ areas within each quadrat.

# 3.4. Data pre-processing

## 3.4.1. Grassland condition: converting a qualitative measure into a quantitative gradient

The partial least square regression (PLSR) model requires a continuous response variable, so using mass (in g) and % cover as grassland variable responses is valid. However, condition, as defined in the UK by the Common Standards Monitoring (CSM) guidance booklets (i.e. National Vegetation Classification, NVC) (JNCC, 2004; 2006) is a qualitative and discrete measure established using grassland type specific criteria. Therefore, instead of pursuing an approach which caters for a range of response variable types (categorical, nominal, etc.) and has options to address multicollinearity such as a penalised generalised linear model (Nelder and Wedderburn, 1972) or a penalised generalised additive model approach (Hastie and Tibshirani, 1986) this condition measure was simply converted to a continuous form for direct use as the response with PLSR.

The seven chosen grasslands were classified using the NVC system, before their condition was determined, as each grassland type has its own set of condition-related criteria in the CSM guidelines. To classify each grassland, species abundance data collected on the ten quadrats established on each grassland were analysed using MAVIS software (Smart et al., 2016) which gave each grassland a NVC category. CSM guidelines (JNCC, 2004; 2006) were then used to determine how closely related each quadrat was to the guidelines for the NVC category of that particular grassland, except for relatively improved grasslands which were compared to the guidelines for MG5 grasslands. Species abundance, % cover of grassland variables and grass height measurements were compared to the NVC-specific condition criteria in the CSM guidelines for every quadrat (summary of criteria provided in Table 3.5). A “good” rating was given for each criterion met or a “bad” rating was given otherwise. For example, if forb cover of 40-90% was a criterion then a “good” rating would be given if forb cover is 50% but a “bad” rating would be given if forb cover is 20%. The good:bad ratio was determined for each quadrat by calculating the ratio of the number of “good” and “bad” criteria. This ratio became resultant CSM-condition variable and had a continuous range from 0 to 1. No weighting was given to particular criteria, so each criterion contributed equally to the good:bad ratio. Each NVC category had a different set of criteria meaning that a different number of criteria were referred to for each target grassland. Furthermore, some guidelines were not used as data were not available for this purpose such as signs of grazing.

*Table 3.5: Provides information related to how the NVC of each quadrat (and therefore each grassland) was determined. This includes the alphanumerical identification code of the criteria that was applied, criteria within that classification that were applied, and criteria that it was not possible to apply because of a lack of data.*

| **Grassland** | **Grassland criteria applied** | **Criteria used** | **Criteria not used** |
|---|---|---|---|
| CG2b | CG2<br><br>10 criteria | >30% and <90% forb cover, <5% scrub cover, <25% dead material cover, <5% bare ground cover, average height >2cm and <50cm, two or more positive indicator species, <20% agricultural species cover and <10% cover by any one agricultural species, <20% cover by rank grasses and sedges plus <10% cover for Arrhenatherum and Dactylis species, <=5% agricultural weeds, no introduced species | Extent, scrub and trees plus bracken, local distinctiveness |
| CG10a | CG10<br><br>8 criteria | <33% forb cover, <10% scrub cover, <10% dead material cover, <10% bare ground cover, <10% *Juncus effuses* cover, <25% *Ranunculus repens* and *Bellis perennis* cover, at least two positive species indicators | Extent, <1% non-native species, grazing indicators |

| | | | |
|---|---|---|---|
| | | present, <1% negative species cover | |
| M19a | M19<br><br>7 criteria | <10% scrub cover, disturbance: <10% bare ground cover plus <10% damaged *Sphagnum* species cover, at least six positive species indicators present, *Sphagnum fallax* is not the only *Sphagnum* species, >50% cover for at least three indicator species, <1% negative species cover, no signs of burning | Extent, indicators of browsing (e.g. shrub grazing), peat erosion, <75% Ericaceous species cover, <1% non-native species |
| MG5b<br><br>MG6b<br><br>MG6c | MG5<br><br>7 criteria | >40 and <90% forb cover, <5% scrub cover, <25% dead material cover, <5% bare ground cover, at least two positive species indicators present, agriculturally favoured species cover and rank grasses and sedges cover: <10% for one species or <20% collectively, <5% agricultural weeds cover | Extent, height |

## 3.4.2. Processing response data before model training

### 3.4.2.1. Test for normality

One assumption made when using a linear regression approach such as PLSR is that there is a normal distribution of errors. Furthermore, the results of PLSR can be considered unreliable if affected by error heteroscedasticity. These issues can be addressed by transforming non-normal response data (Meyer et al., 2019; Ripley et al., 2019). As many of the grassland variable data sets appeared to be skewed based on a subjective assessment of distribution graphs, a Shapiro-Wilk test for normality was applied to quantitatively assess whether the distribution of each data set was normal.

The W value is calculated as:

$$W = b^2 \div SS \qquad (eq.\ 3.1)$$

Where:

$$b = \sum_{i=1}^{m} a_i (x_{n+1-i} - x_i) \qquad (eq.\ 3.2)$$

With m being n ÷ 2 if n is even, or (n-1) ÷ 2 if n is odd, and:

$$SS = \sum_{i=1}^{n} (x_i - \overline{x})^2 \qquad (eq.\ 3.3)$$

The closer the W value is to 1, the more normal the distribution is considered to be although it is possible for values >0.95 to be applied to distributions that are clearly non-normal subject to the sample size (Shapiro and Wilk, 1965). A p-value (probability associated with W value) is also calculated, where the null hypothesis of normal data distribution is rejected if p<0.05. In the context of this thesis, response data were considered to be significantly skewed if the results of a Shapiro-Wilk test (Shapiro and Wilk, 1965) produced a p-value of <0.05 (i.e. at the 95% level).

A one sample Kolmogorov-Smirnov test, Lillefors test or an Anderson-Darling test could have been used for the same purpose (Razali and Wah, 2011). The one sample Kolmogorov-Smirnov test and related Lillefors test compares the distribution of a given data set against an ideal normal distribution with the null hypothesis that the data set being analysed is from a normally distributed population. This is achieved by calculating the observed values against the expected cumulative relative frequencies that would exist if the data set followed an ideal normal distribution. The Kolmogorov-Smirnov test and Lillefors test differ in the calculations made in determining whether the null hypothesis is rejected. The Anderson–Darling test evaluates whether a sample comes from a defined distribution, which in this context is a normal distribution (Razali and Wah, 2011). Although all tests achieve the same purpose and had no clear advantage in the context of this study, the Shapiro–Wilk test was chosen as it is considered to be the most powerful (Razali and Wah, 2011).

One disadvantage of all aforementioned tests is that they are less powerful on small sample sizes, where the term “small sample sizes” has not been quantified. Therefore, it is not clearly defined whether the sample sizes used in this study constitute “small sample sizes”. It has been stated that the Shapiro–Wilk test requires relatively few samples to give reliable results but the recommendation is to use at least 50 samples (Razali and Wah, 2011) while Royston (1995) explains that any sample size between 3 and 5000 is viable for analysis using the Shapiro–Wilk test. This study used less than 50 samples for most analyses (10, 30, 40 or 90) where the Shapiro-Wilk test was still the more powerful than comparable tests (Razali and Wah, 2011) but it was not made unambiguously clear if this sample size is sufficient for reliable results in this particular study. Also, the Shapiro–Wilk test is known not to work well in samples with many identical values (Shapiro and Wilk, 1965). This was the case when using bare ground for all grasslands and CSM-condition for Grasslands 1 and 6 as response variables in this thesis for example.

#### 3.4.2.2. Transformation of response variables

Response data that were not considered to have a Gaussian distribution after a Shapiro-Wilk test were transformed before PLSR analysis to help address the assumption of a normally distributed error term made by the PLSR analyses and to address the issue of error heteroscedasticity. A log transformation was applied to the response data if the response distribution was right- or left-skewed respectively, where left-skewed response data were “reflected” before transformation (Meyer et al., 2019; Ripley et al., 2019). Compositional data were also log transformed to remove the constraints on data (i.e. 0-100% for cover data) and to account for the non-linear relationship between spectral data and the condition-related variables chosen for this thesis. An optimising constant (c) was included to optimise the transformation by taking the extent of the skew into consideration (Meyer et al., 2019; Ripley et al., 2019). The equation is:

$$log(x + c) \quad \text{(eq. 3.4)}$$

Although log transforming compositional data helps deal with issues related to using compositional data in regression analyses, using a log ratio transform before regression (Aitcheson, 1982) or using beta regression (Douma and Weedon, 2018) would be a more effective but less generic approach to transforming response data.

## 3.4.3. Grassland reflectance

### 3.4.3.1. CROPSCAN data processing

Incoming and reflected irradiance data were collected by the CROPSCAN, then converted to millivolt quantities which were stored in the data logger. To calculate percent reflectance, the software makes sensor sun angle cosine corrections and temperature corrections to the millivolt readings. Corrections for temperature are necessary as dark readings (millivolts with no irradiance) and responsivity (millivolts per watts/$m^2$ of irradiance) are affected by differences in temperature. Cosine corrections are made to account for the sun angle using information on date, time, latitude and longitude. The end product of converting and correcting raw millivolt data is a CSV file with reflectance values for each of the sixteen bands collected at each data with associated dates and times of data collection (CROPSCAN Inc., 2018).

Some of the spectral data collected with the CROPSCAN during the spring fieldwork campaign used an incorrect hardware setup meaning that the spectral data were incorrectly calibrated. To account for this, data were collected using a CROPSCAN with the correct and the same incorrect setup used in Parsonage Down along the same 50m transect on a grassland in Oxfordshire (UK). The two spectral data sets were then compared to see if there was a consistent difference between comparable bands along the transect. As the spectral data collected on the same transect was consistently different between the correct and incorrect setup, a coefficient was calculated on each wavelength by calculating the difference in reflectance between the correct and incorrect setup. This coefficient was then applied to the incorrectly calibrated CROPSCAN data collected during spring at Parsonage Down NNR.

#### 3.4.3.2. ASD data processing

Binary files were converted to ASCII files, then absolute reflectance calculated for each band on each data point using white reference data for calibration using Excel with prepared macros provided by the Field Spectroscopy Facility. The water absorption bands (1350-1460nm and 1790-1960nm) were then removed as these bands have a signal to noise ratio too low for these data to be viable. After this, it was found that the integrity of these data had been compromised by the difficult weather conditions experienced at Ingleborough NNR so it was decided not to use these spectral data in analysis.

#### 3.4.3.3. SVC data processing

Raw data collected using the SVC were saved in the device as .sig files. An Excel spreadsheet with prepared macros was provided by the Field Spectroscopy Facility to calculate absolute reflectance for each measurement using paired white reference and target data. These calibrated reflectance values for 1024 bands are then interpolated across the spectral range of 350-2500nm to produce a reflectance spectral signature for every nanometre in the 350-980nm range and every two nanometres in the 980-2500nm range. Then the atmospheric water absorption bands were removed (1350-1520nm & 1790-1960nm) due to their low signal to noise ratio, leaving 1249 bands.

### 3.4.3.4. Rikola VNIR imagery processing

To prepare the Rikola VNIR imagery for analysis, several processing steps were necessary; which included pre-processing (calibration), georeferencing the images, normalising the images for illuminance, calculating reflectance, autoscaling the reflectance values then extracting the reflectance values for analysis.

#### *Pre-processing (calibration)*

Multispectral images collected using the Rikola camera were calibrated using Rikola Hyperspectral Imager v2.1 software. Readings were taken from a black reference panel prior to each flight, which was used as a dark reference that the drone images were calibrated against. The results of pre-processing were stacks of multispectral images of reflected irradiance values, each image representing data collected on a wavelength.

#### *Georeferencing*

As a drone collects images on a target grassland, data on each band are not collected simultaneously for each image meaning that these bands are not georeferenced against each other. The georeferencing of images is necessary to ensure that spectral data truly represent a particular space such as a quadrat. Firstly, Environmental for Visualising Images (ENVI) software was used to separate each multispectral image into 30 mono-band images. ArcGIS v10.6 was then used to align the 30 images to each other. These images were then “stacked” to produce a georeferenced multispectral image.

#### *Normalising illumination*

Despite drone imagery being collected at Parsonage NNR in clear sky conditions within two hours of solar noon, some parts of the drone imagery had far higher illuminance relative to other parts of the imagery. This within-image variance in illuminance is related to the solar zenith angle and the view angle of the camera (Roy et al., 2016) and can make the results of regression analysis erroneous as the predicted response values can simply be a reflection of illuminance values. To ensure the integrity of the results of PLSR statistical modelling, images were normalised against a column of pixels that represented the average illuminance for the image using R software (v. 3.5.1).

### *Calculating reflectance values*

R software (v. 3.5.1) was used to calculate the reflectance of each pixel value (radiance) for all images. As reflectance is the proportion of radiation not absorbed or transmitted, the following equation was applied to each pixel value:

$$P_{ref} = P_{rad} \div R_{rad} \times R_{ref} \qquad (eq.\ 3.5)$$

Where $P_{ref}$ refers to pixel reflectance, $P_{rad}$ refers to pixel radiance, $R_{rad}$ refers to radiance from a reference panel and $R_{ref}$ refers to reflectance from a reference panel. Reference panel readings were taken using a SVC on a grey panel.

### *Extracting quadrat reflectance data from the images*

To train PLSR statistical models using spectral reflectance as predictors, reflectance values calculated from Rikola imagery had to be extracted from each quadrat. Once the processing of Rikola images had been completed to produce georeferenced pixels of reflectance values, reflectance values were extracted from all 30 quadrats set up in Parsonage Down NNR during the summer fieldwork campaign. Using ENVI software, a “region of interest” was established on top of each 1m$^2$ quadrat which calculated the average reflectance values for each band using all of the 6cm$^2$ pixel values within. These average values were extracted for use as training data for PLSR statistical models. Taking the average value was considered to be the simplest viable approach and the most comparable with other literature, but other calculations can be utilised instead such as the variation, maximum value and minimum value.

#### 3.4.3.5 Scaling of reflectance data

Prior to applying PLSR, autoscaling was used to scale spectral reflectance data to a mean of zero and a standard deviation of one at each spectral band (Farrés et al., 2015; Wold et al., 2001) for data collected with all spectral devices used in this thesis. Autoscaling is defined as:

$$\tilde{x}_{ij} = \frac{x_{ij} - \bar{x}_i}{s_i} \quad (\textit{eq. 3.6})$$

Where the average of all spectral values for a quadrat is taken away from the spectral value, then this value is divided by the standard deviation of all spectral values for a quadrat to get the autoscaled value. Autoscaling addresses assumptions made when using PLSR (Farrés et al., 2015; Wold et al., 2001) by de-emphasizing the relatively higher and highly variable values in the near and short wave-infrared regions of the EM spectrum (van den Berg et al., 2006; Haaland and Thomas, 1988) and also prevents the results of the VIP analyses (explained in Section 3.5.2.1) from being biased. One alternative is to use range scaling which is sensitive to outliers. Another option is Pareto scaling which is sensitive to large fold changes, i.e. differences between the values of the predictors.

## 3.5. Analytical methods

The overarching approach (summarised in Figure 3.7) was to apply partial least squares linear regressions between grassland reflectance, grassland variables and condition data to explore the strength of the relationships between (1) grassland reflectance and grassland CSM-condition, (2) grassland reflectance and grassland variables and (3) grassland variables and grassland CSM-condition. This approach was designed to establish if there is a consistent relationship between grassland reflectance and grassland CSM-condition and which of the chosen grassland variables are more likely to contribute to this relationship. In other words, can grassland variables form the basis for remotely sensed based approaches to monitoring grassland condition? And which grassland variables are the most suitable?

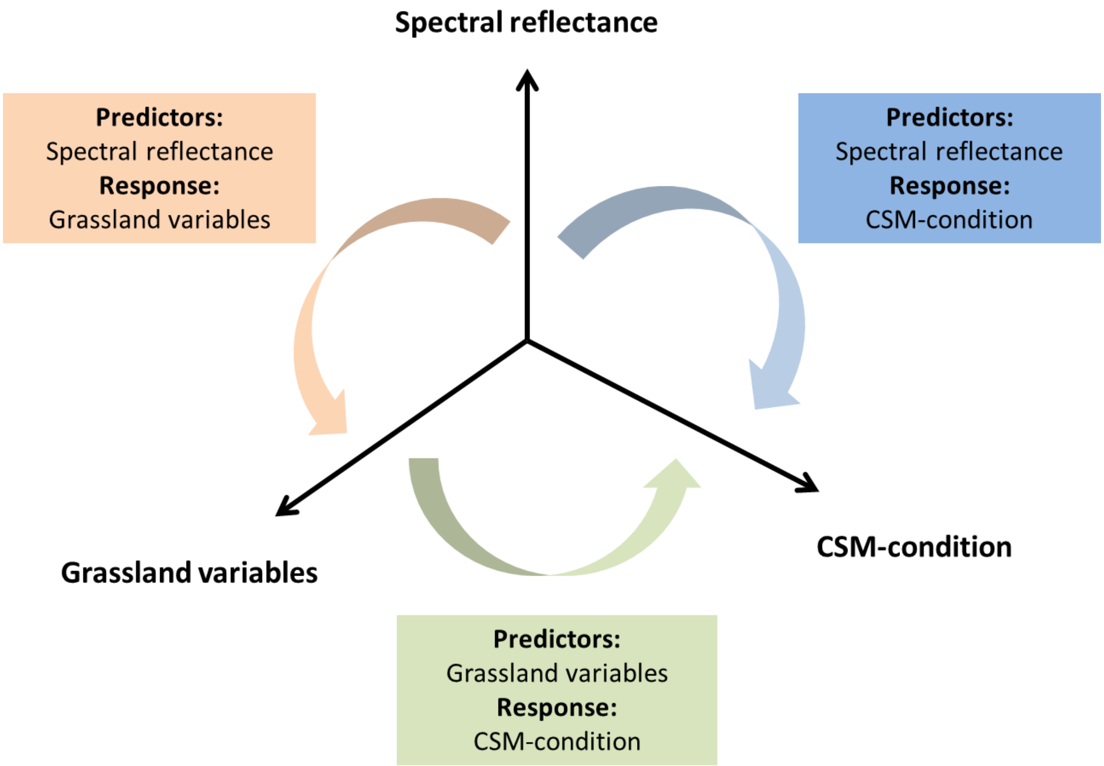



*Figure 3.7: Schematic of overarching approach used to establish if remote sensing can be used to determine grassland condition and to identify which spectral bands and which grassland variables are particularly suited for condition monitoring using remote sensing.*

### 3.5.1. Testing for significant difference of grassland variables between grassland sites

Botanical experts provided support in selecting the target grasslands, one reason for selecting them is that the grasslands should be as different in their characteristics as possible to represent a range of different grassland types. It was hypothesised that these different characteristics would be reflected in significantly different quantities of grassland variables. For example, an undergrazed acid mire grassland will have significantly different quantities of graminoids compared to an overgrazed alkaline grassland. A Wilcoxon rank sum test (a.k.a. Mann-Whitney U test) (Bauer, 1972) is a non-parametric test for significant difference between the medians of two independent data sets. This method was used to establish whether there were significant differences between grassland sites in terms of the grassland variable distributions. Differences were considered significant if $p <= 0.05$ (i.e. at the 95% level). A non-parametric method was chosen as almost all of the mass and % cover data sets were found to have a non-normal distribution by the Shapiro-Wilk test (Whitley and Ball, 2002). The two-sided version of the test does not suggest the directionality if two data sets are deemed to be different, which was considered advantageous when dealing with a combination of left-skewed and right-skewed data. This approach was chosen as the data sets being compared were not matching (as the data being compared was collected on different grasslands), ruling out the use of analyses such as the Sign test or Wilcoxon Signed Rank Test (Whitley and Ball, 2002). Also, data sets were compared against each other (i.e. between two grasslands) meaning that analyses that compare groups of data sets and produce one result such as a Kruskal-Wallis test were not considered appropriate.

Boxplots showing the mass or % cover of grassland constituents for each grassland were produced to visualise the differences in distribution. To test for significant differences in the values of each grassland variable between different grasslands, an unpaired two-sample Wilcoxon test was applied using R software (version 3.4.2 or 3.5.1). This non-parametric method, which compares the medians of each data set, can be applied to skewed data to compare two independent groups of samples. The equation is as follows:

$$U_1 = n_1 n_2 + n_1(n_1 + 1)2 - R_1 \qquad (eq.\ 3.7)$$

And:

$$U_2 = n_1 n_2 + n_2(n_2 + 1)2 - R_2 \qquad (eq.\ 3.8)$$

Where n is the sample size and R is the sum of ranked values. The smaller of the U values from the two sets of samples is chosen. A U value closer to zero suggests that the null hypothesis can be rejected, but this can only be done after comparing the U value against a table of significant U values. The significant U value depends on the sample size and the alpha value chosen (default is 0.5 which is the equivalent of the 95% level). If U is equal to or less than the significant U value then the null hypothesis, which in this case is that the mass or % cover of grassland variables between two grasslands is not significantly different, can be rejected.

### 3.5.2. Partial least squares regression

In the context of this thesis, multicollinearity can occur when spectral bands or grassland variable values (i.e. predictors) can be predicted to a high degree of accuracy by other spectral bands or grassland variables. The use of redundant variables (i.e. multicollinear variables) increases the likelihood of model overfitting (Wold et al., 2001)**.** Therefore, it was deemed important to consider a statistical modelling approach that helps deal with the issues of multicollinearity and model overfitting.

Firstly, to test whether a predictor decomposition approach such as PLSR was necessary, correlation matrices were produced to test the strength of multicollinearity between predictors. It was deemed that an approach such as PLSR would be necessary to deal with multicollinearity if there were any significant correlations. This is important as weak correlations would suggest a PLSR methods would not be worth following and a less complex modelling approach such as an ordinary least squares (OLS) regression would suffice (i.e. standard regression). Results were considered significant if the correlation coefficient value (r) came within the ranges of $r > +0.8$ or $r < -0.8$ and was accompanied with by a P value $\leq 0.05$.

As it was deemed necessary to choose a method that helped overcome the issues of multicollinearity and overfitting (See Figure 4.1, Section 4.4.1); partial least squares regression (PLSR), also called projection of latent structures regression, was chosen for analysis. PLSR (Wold et al., 2001) decomposes the predictor and response data sets simultaneously into relatively few orthogonal components (latent variables) that explain as much of the covariance between predictors and responses as possible. A linear regression step then uses these components to predict the responses.

The latent variables can also be referred to as X-scores which predict Y and model X. X-scores can be denoted as $t_a$ where a = (1, 2...A) and A is the number of X-scores. They are estimated as linear combinations of the original variables $x_k$ with the weighting coefficients $w_{ka}$ where k = (1...K) and K is the number of X variables. The equation for $t_a$ (or $t_{ia}$ for one indexed object) is:

$$t_{ia} = \sum_k W_{ka} X_{ik} \qquad (eq.\ 3.9)$$

The X-scores are multiplied by the loadings $p_{ak}$, which should represent good summaries of X:

$$X_{ik} = \sum_a t_{ia} p_{ak} + e_{ik} \qquad (eq.\ 3.10)$$

Where $e_{ik}$ represents the X-residuals, which should be relatively small if the loadings ($p_{ak}$) genuinely represents a good summary. To calculate the multivariate Y ($y_{im}$), Y-scores ($u_a$) are multiplied by the weights $c_{am}$, $g_{im}$ represents the Y-residuals:

$$y_{im} = \sum_a u_{ia} c_{am} + g_{im} \qquad (eq.\ 3.11)$$

The X-scores are used as predictors of Y as follows:

$$y_{im} = \sum_a c_{ma} t_{ia} + f_{im} \qquad (eq.\ 3.12)$$

The Y-residuals ($f_{im}$) express the deviations between the observed and modelled responses. Because of Eq. 3.9, Eq. 3.12 can be rewritten to look like a multiple regression model:

$$y_{im} \sum_a c_{ma} \sum_k w_{ka} x_{ik} + f_{im} = \sum_k b_{mk} x_{ik} + f_{im} \quad \text{(\textit{eq. 3.13})}$$

The PLS-regression coefficients ($b_{mk}$) can be written as:

$$b_{mk} = \sum_a c_{ma} w_{ka} \quad \text{(\textit{eq. 3.14})}$$

These coefficients are used to calculate the fitted value(s) of the response variable.

One advantage that PLSR has over regression methods that use PCA regression, or a similar approach, is that PCA regression produces components from predictors that explain as much of the variance of the predictors as possible before regression analysis but does not utilise response data to establish the best way to predict as much of the variance of the response data as possible. Another advantage to using PLSR is that this analysis can be followed by a variable importance in projection (VIP) analysis to determine which variables are most important in predicting the response values. Spectral data were autoscaled (explained in Section 3.4.3.5) before analysis. Although there are few studies that compare VIP to similar analyses, Farrés et al. (2015) found that VIP projections were easier to interpret than selectivity ratio projections (another test to ascertain which variables are most important in predicting the response values, which is calculated as the ratio between the explained and the residual (unexplained) variance for each variable) when dealing with mass spectrometry data.

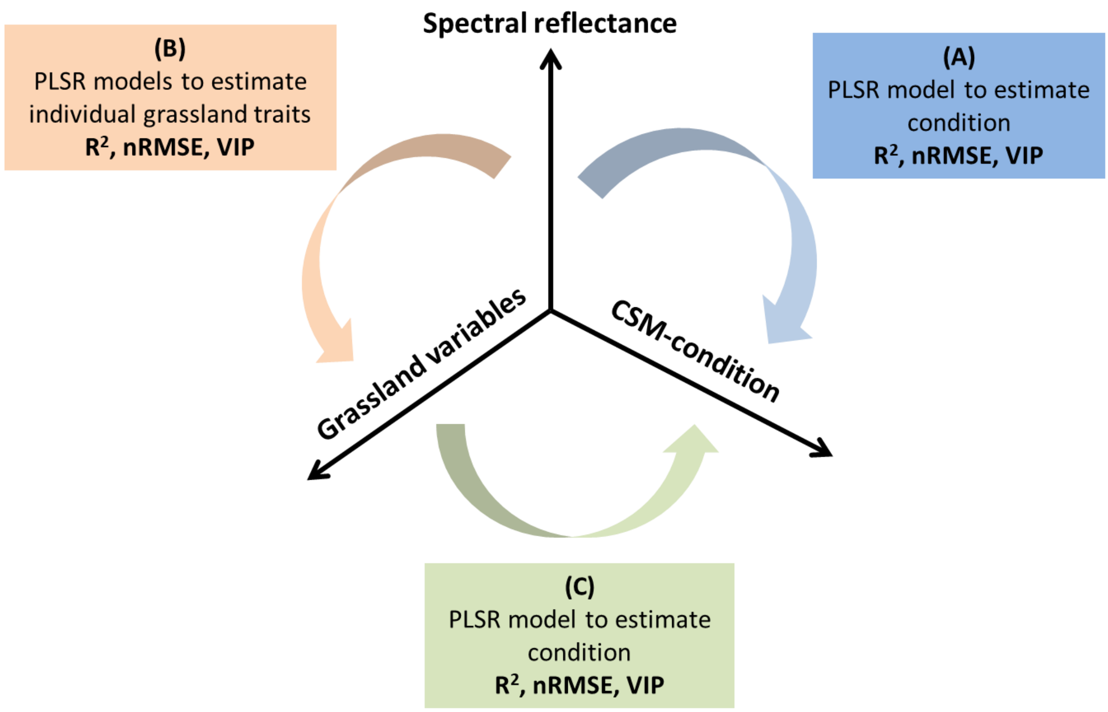



*Figure 3.8: Schematic showing the partial least squares regression (PLSR) approach developed to establish if spectral data can be used to determine grassland condition (A) and to identify which spectral bands (B) and which grassland variables (C) are particularly suited for condition monitoring using spectral remote sensing. $R^2$, normalised root mean square error (nRMSE) and variable importance in projection (VIP) are used to evaluate and compare model performance.*

PLSR (Mevik et al., 2019; Wold et al., 2001) was used to assess the ability of spectral data to predict grassland variables and CSM-condition (A and B in Figure 3.8), plus the ability of grassland variables to predict CSM-condition (C in Figure 3.8). The coefficient of determination ($R^2$) is an 'in-sample' measure that represents the % of variance of the response variable explained by the regression model, and a leave-one-out cross validation root mean square error (RMSE) is an alternative 'out-of-sample' measure of the accuracy of the model (Wold et al., 2001). This thesis used adjusted $R^2$, which compensates for the addition of predictors by only increasing if the new latent variable enhances the model more than what would be expected by chance, which is defined as:

$$R_{adj}^2 = 1 - \left(1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}\right) \frac{n-1}{n-p-1} \qquad (eq.\ 3.15)$$

Where y represents the measured values, ŷ represents the predicted values, ȳ represents the average measured value, p represents the total number of explanatory variables in the model and n represents the number of samples. To make the performance of different PLSR models comparable, RMSE was normalised (nRMSE):

$$nRMSE = 100 \frac{\frac{1}{N}\sum_{i=1}^{N} (S_i - O_i)^2}{sd(O_i)} \qquad (eq.\ 3.16)$$

Where S refers to the predicted values and O refers to the observed values. This made different model runs comparable (Bigiarini, 2019). $R^2$ and nRMSE were used to compare model performance between grassland sites. $R^2$ results were considered strong ($R^2$>0.7), moderate ($R^2$ of 0.5-0.7) or weak ($R^2$<0.5) based on previous literature (Capolupo et al., 2015; Doughty et al., 2011; Roelofsen et al., 2014) whilst models with nRMSE >100 were considered weak as models with this level of prediction accuracy using true data are no more accurate than a model using randomised data. Higher $R^2$ values and lower nRMSE values were considered to be indicative of a better performing PLSR model. A linear regression approach to predicting grassland variable values may underestimate the largest (Psomas et al., 2011) or smallest values (Chen et al., 2009) as the relationship between spectral data and grassland variables may not be linear.

There are other analytical methods that help deal with overfitting and multicollinearity. A few predictors can be manually selected (e.g. vegetation indices) or selected through other analyses to reduce multicollinearity and make overfitting less likely. This can be achieved by decomposing predictors into relatively few components prior to regression (e.g. PCA) or by applying methods that incorporate the use of latent variables other than PLSR such a penalised generalised additive modelling approach (Dormann et al. 2013).

#### 3.5.2.1. Variable Importance in Projection

Variable Importance in Projection (VIP) coefficients can be used to calculate the relative contribution of each predictor when predicting the responses (Farrés et al., 2015; Wold et al., 2001). Farrés et al. (2015) defined the VIP score for $j^{th}$ variable as:

$$VIP_j = \sqrt{\frac{\sum_{f=1}^{F} w_{jf}^2 . SSY_f . J}{SSY_{total} . F}} \qquad (eq.\ 3.17)$$

Where $VIP_j$ is a measure of the global contribution of j variable in the complete PLSR model, $SSY_{total}$ is the total sum of squares explained of the responses, F is the total number of components, $w_{jf}$ is the weight value for j variable and f component and squaring this is considered to give the importance of the $j_{th}$ variable in each $f_{th}$ component, $SSY_f$ is the sum of squares of explained variance for the $f_{th}$ component and J number of X variables. A more detailed explanation of the methods of VIP has been provided by Wold et al. (2001) and Farrés et al. (2015).

In the context of this study, VIP was used to identify key spectral bands for predicting grassland variables plus condition (A and B in Figure 3.8) and key grassland variables for predicting grassland condition (C in Figure 3.8). Spectral bands or grassland variables with VIP coefficients => 1 were considered to be important (Farrés et al., 2015).

#### 3.5.2.2. Model fit and validation

Leave-one-out cross validation (LOO-CV) was used to test the predictive ability of each model (Mevik et al., 2019; Wold et al., 2001) where the RMSE values were derived from LOO-CV then normalised (nRMSE) so that PLSR models were directly comparable. To avoid overfitting, the number of latent variables (referring to the PLSR components derived from the spectral bands) for each model run was determined by the lowest prediction error sum of squares (PRESS) value.

For each predictor to response combination, model validation was established by calibrating a PLSR model *m* times where 80% of the quadrat data used for training was chosen randomly for each model run. To establish *m*, first the binomial coefficient was used to establish the maximum number of iterations of 80% of the quadrat data without repetition or replacement for each combination of grasslands:

$$m = \frac{n!}{r!(n-r!)} \qquad (eq.\ 3.17)$$

Where in this context *n* is the number of quadrats and r represents the sample size which is set to 80%. Where analyses were conducted on individual grasslands (i.e. *n* = 10 and *r* = 8), *m* = 45 but where grasslands were analysed collectively (such as where all three Parsonage grasslands were analysed collectively), *m* was considered to be too large to make computing the results realistic so *m* was limited to 1000 for these analyses.

As the variance in the training data means that there will also be variance in the fitted models, the median of the resulting 45 or 1000 $R^2$ and 45 or 1000 nRMSE values from the iterated PLSR model runs were used as the final results (i.e. a form of bagging (Breiman, 1994), these will be called the iterated model runs or iterated results from now on) to account for this variance and reduce the chance of overfitting. A non-parametric method was used to calculate 99% confidence intervals of the $R^2$ and nRMSE results to capture the variability of the iterated model runs (see Section 3.5.2.3) (Campbell and Gardner, 1988).

To establish if the resulting PLSR models (referred to as actual models) provided predictions that are more accurate to that found by chance in a random case (referred to as random models), PLSRs were run 44 or 999 more times for each predictor to response combination, but with the response variable values randomly assigned to a different set of predictors (referred to as random models). Then, the median result of the actual models were ranked against the results of the 44 or 999 random models to establish its place in this ranking. If the actual model results were placed in the top 5% most accurate fits, in this case where the results placed in position 950 or above where *m* = 1000, then the actual model $R^2$ or nRMSE values can be said to be significant at the 95% level.

#### 3.5.2.3. Confidence intervals (CIs)

Confidence intervals can be used to determine a range of values that have a set probability (usually 95% chance) of including the population median. The following equation was used to calculate the lower and upper confidence intervals:

$$(n \div 2) - 2.58 \times \left(\sqrt{n} \div 2\right) \qquad (\textit{eq. 3.18})$$

$$1 + (n \div 2) - 2.58 \times \left(\sqrt{n} \div 2\right) \qquad (\textit{eq. 3.19})$$

In this study, confidence intervals were calculated with 99% confidence to capture the variability of the iterated PLSR runs meaning that there is a 1% chance that the population median would be outside of the calculated range of values. A relatively narrow CI range suggests greater precision of the sample statistic as an estimate of the overall population value (Campbell and Gardner, 1988). In the context of this study, a narrower CI range suggests that the median value of the iterated PLSR runs is more representative of all 45 or 1000 results. In other words, the distribution of the iterated $R^2$ and nRMSE results is relatively narrow.

#### 3.5.2.4. Coefficient of variation

To test the stability and consistency of the PLSR model runs, the coefficient of variation (CV) was calculated for all of the model runs for each grassland variable and for CSM-condition to highlight which of these responses produced the most consistent (strong or weak) $R^2$ and nRMSE results. The equation for calculating CV is:

$$CV = \frac{\sigma}{\mu} \times 100 \qquad (\textit{eq. 3.20})$$

In practical terms, this approach would highlight any grassland variables including CSM-condition that could be consistently predicted (or not predicted) across grasslands, seasons and when using different spectral devices.

# 3.6. Summary of the main chapters

Where and when spectral data were successfully collected, and with which devices, influenced which data sets were utilised for each of the main chapters in this thesis. While the main analytical approach remained the same, reflectance data were combined in different ways with the other data sets in the next three chapters. Table 3.6 summarises the main characteristics of each study.

*Table 3.6: Summarises some of the characteristics of the data sets used in the main chapters of this thesis. This includes where data were collected, which season, which spectral devices were used and the scale of the data collection.*

| Chapter | Locations | Seasons | Spectral devices | Sample sizes (n) | Scale |
|---|---|---|---|---|---|
| Chapter 4 | Ingleborough NNR<br>Parsonage NNR | Summer-Jun'17<br>Summer-Jun'18 | CROPSCAN* | 10, 30, 40 or 70 | $1m^2$ |
| Chapter 5 | Parsonage NNR | Spring-Apr'18<br>Summer-Jun'18<br>Autumn-Sep'18 | CROPSCAN* | 10, 30, or 90 | $1m^2$ |
| Chapter 6 | Parsonage NNR | Summer-Jun'18 | CROPSCAN*, Rikola camera & and SVC + | 10 or 30 | $1m^2$ and 200x1m |

*CROPSCAN data were successfully collected during the summer 2017 at Ingleborough NNR and during 2018 for all three seasons at Parsonage NNR.

+ During summer 2018, good quality SVC spectral data were collected at Parsonage NNR, on 28 of 30 quadrats.

& Good quality Rikola camera imagery was also collected during summer 2018 at Parsonage NNR.

All three studies utilised traditional (mass, % cover) data and CROPSCAN spectral data collected on three grasslands at Parsonage Down NNR during the summer season. All studies also used PLSR, VIP and CV to understand which grassland variables (including CSM-condition) can be predicted with a reasonable level of accuracy and precision using scaled spectral data as predictors plus whether unscaled grassland variables can predict CSM-condition with acceptable accuracy and precision (Question 4, see Section 1.2 for list of questions). The impact of using mass or % cover variables on the results was also investigated across all three studies (Question 5). In addition, all models trained in each study were compared with models trained with randomised data to test if the models have stronger predicting power than models trained with randomised data.

VIP was used to understand which spectral bands, when used as predictors, had predictive power considered significant (VIP => 1) when predicting grassland variables and CSM-condition, plus which grassland variables had significant predictive power when predicting CSM-condition (Questions 6 and 8). One reason for this analysis was to help establish whether access to reflectance recorded across a broader range of the spectrum, where SWIR spectral values are included, instead of only utilising the visible and near-infrared (NIR) spectrum to successfully predict grassland variables and CSM-condition.

The first study (Chapter 4) also uses data collected on four grasslands at Ingleborough NNR during the summer, meaning that data from seven grasslands within the summer season were analysed. This study was conducted to investigate (Question 1) whether the chosen grassland variables form the basis for RS- based grassland condition monitoring and, related to this, whether these grassland variables are the most suitable for estimating grassland condition on a range of different grassland types? The second study (Chapter 5) uses data collected during spring, summer and autumn on three grasslands at Parsonage Down NNR, to investigate (Question 2) the relationship between reflectance and grassland variables plus CSM-condition across the growing seasons. This study also explores which time of the year is most effective for RS based CSM-condition monitoring or if using reflectance data from three seasons would be more effective. The third study (Chapter 6) consists of two parts. The first part compliments the VIP analysis by comparing the predictive power of models trained with spectral data from three different spectral devices (Questions 3 and 7). The second part tests whether models trained with data from all three grasslands and using CROPSCAN data as predictors can be extrapolated from patch level (1m$^2$) to field level (200x1m).

### 3.6.1. Varying sample information within and across sites

In order to assess the effects of combining datasets and how sample size may change results, while at the same time potentially contaminating the PLSR fit with data representing different processes as a consequence of using data from different grassland types, the PLSR models were fitted using combined data. For the first study (Chapter 4), these data consisted of: (1) both locations (where all seven grassland sites are analysed together: 70 quadrats), (2) one NNR location at a time (analysing data from four Ingleborough NNR sites: 40 quadrats or three Parsonage NNR sites: 30 quadrats), and (3) each individual grassland site (analysis of 10 quadrats in each of the seven sites). Thus sample size is one of $n$ = 10, 30, 40 or 70. For the second study (Chapter 5), the PLSR models were fitted using combined data consisting of all three grasslands collectively (30 quadrats per season) and each individual grassland site (10 quadrats per season). Also, PLSR models were fitted with data from all three seasons (30 quadrats per grassland, 90 quadrats for all grasslands) or from one season (10 quadrats per grassland where data were collected during spring, summer or autumn). Therefore, the sample size is one of $n$ = 10, 30, or 90. For the third study (Chapter 6), PLSR models were fitted with data from all three Parsonage sites or each individual grassland site ($n$ = 10 or 30).

## 3.7. Summary of the methods

This chapter has provided details of the approach taken in this thesis to assess the condition of grasslands using RS techniques, addressing each of the questions specified at the beginning of this chapter. Grasslands were defined in the context of this thesis and a description of the study sites provided. Details were also provided on which data sets were collected, how those data were collected and how those data were analysed.

To address Questions 1, 2 and 5 posed in Section 1.2, data were collected from seven grassland sites across two locations that represent a range of grassland types, grazing regimes and improvement levels; data were successfully collected over three seasons on three grasslands at Parsonage NNR and during the summer on four grasslands at Ingleborough NNR. On each of these seven grasslands, a 200m transect was set up and ten quadrats ($1m^2$) placed along it at random. On each quadrat, the following data sets were collected then utilised in analysis: species abundance, the mass and % cover of grassland variables, grass height and spectral data. Species abundance, the % cover of grassland variables and grass height were used to define a quantitative metric considered representative of grassland condition which was labelled “condition”. To address Question 3, a CROPSCAN was used to collect spectral data along the entirety of each transect (200 x $1m^2$ grass patches) and a UAV-mounted Rikola VNIR camera collected multi-band imagery on all seven grasslands

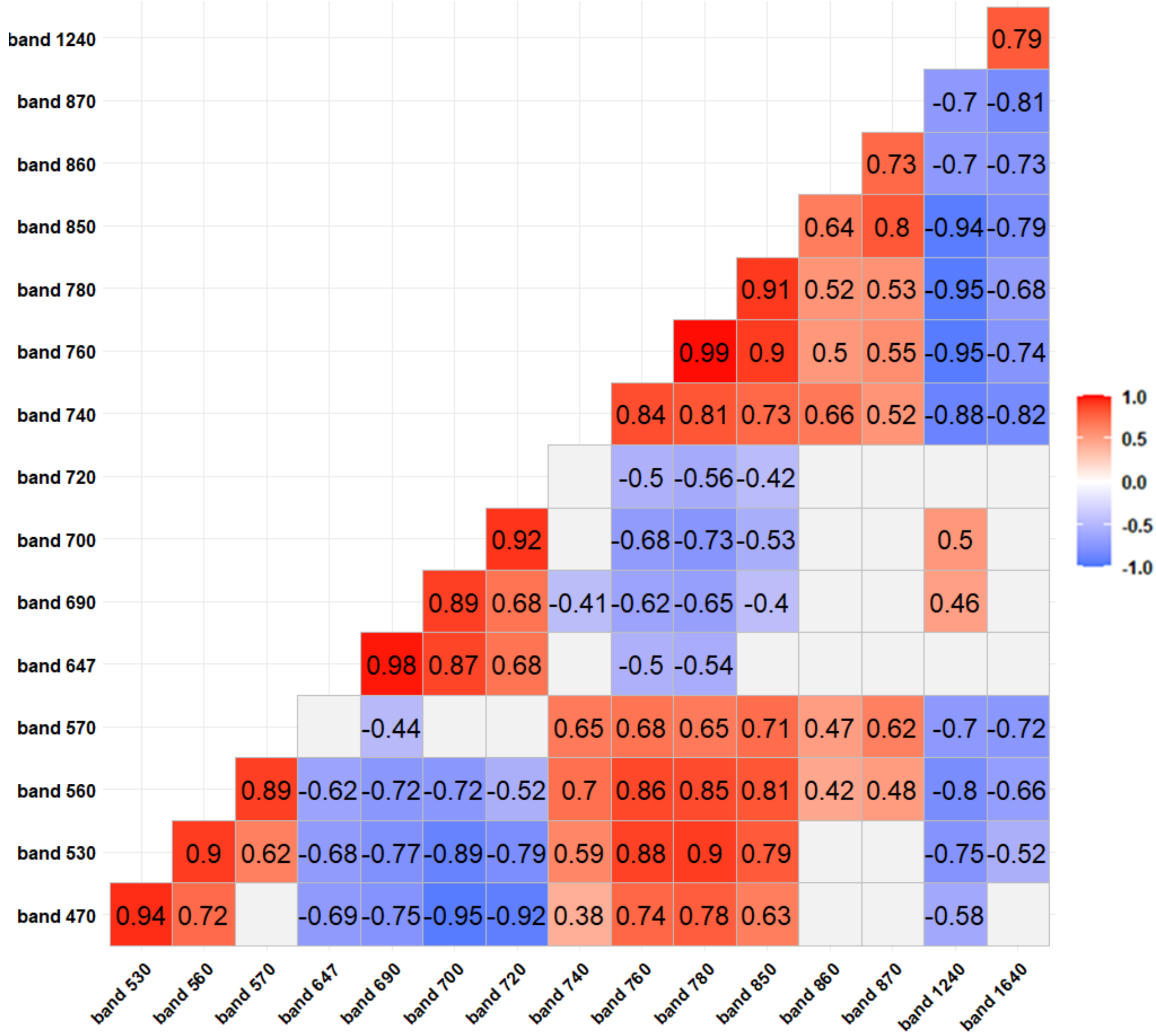
To address Questions 4 and 5, PLSR was used to assess the link between spectral data (predictors) and grassland variables including CSM-condition (responses) plus the link between grassland variables (predictors) and CSM-condition (response). When spectral data were used as predictors; different spectral devices were used, or the SWIR part of the spectrum was removed before analysis, to test whether using the full spectral range made available by some spectral devices is required to successfully monitor grassland condition (addressing Questions 6 and 7). VIP was used to highlight which spectral wavelengths were significantly important in predicting grassland variables including CSM-condition plus which grassland variables were significantly important in predicting CSM-condition (addressing Question 8). The CV for the iterated model runs identified which grassland variables including CSM-condition could be consistently predicted (or not predicted) across grasslands, seasons and when using different spectral devices.

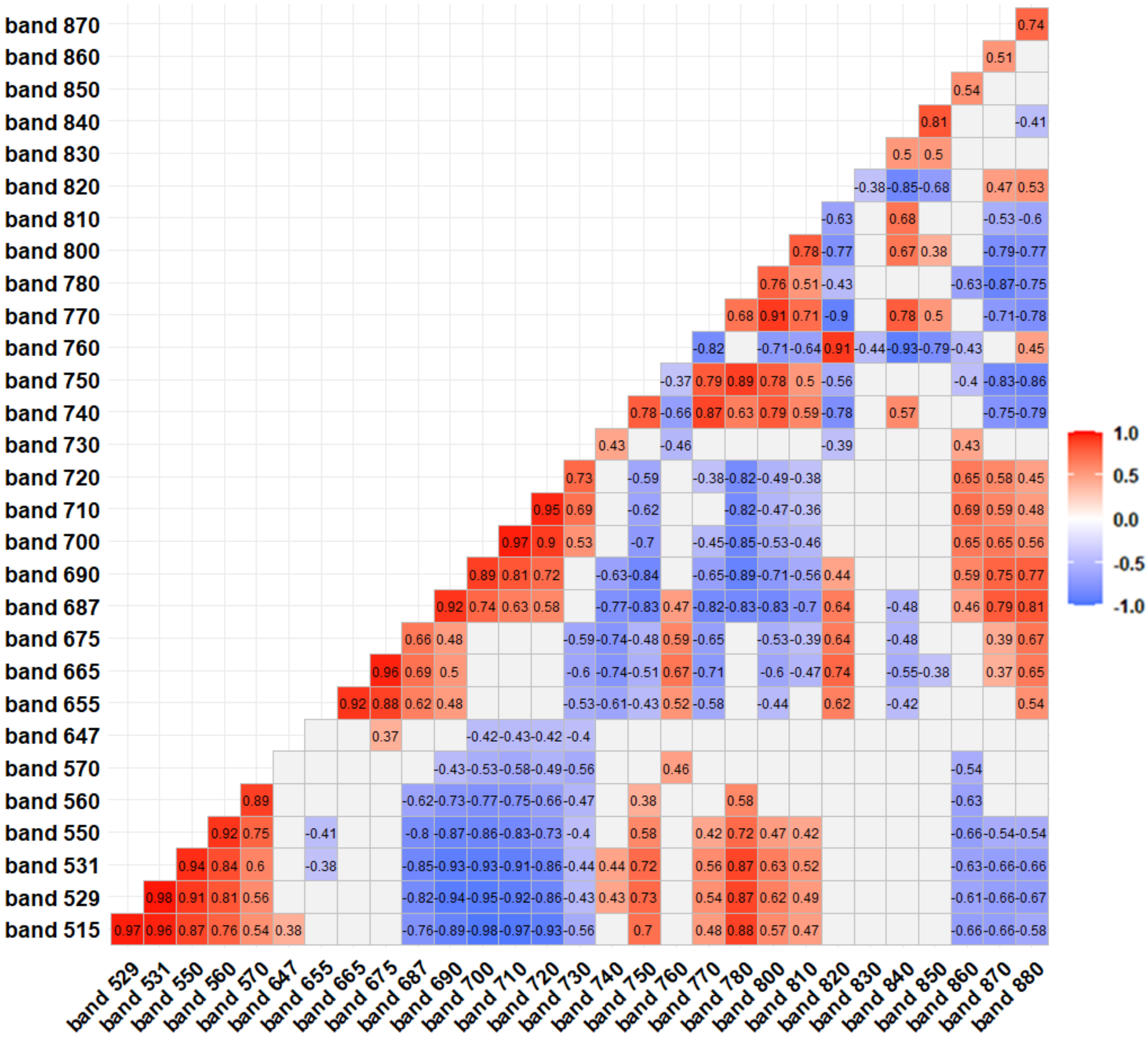
# Chapter 4 - Assessing the condition of semi-natural grasslands using CROPSCAN field radiometry at patch level ($1m^2$)

## 4.1. Predictor correlation matrices

Correlation matrices (Figure 4.1 and Appendix Figures 1 and 2) were produced to investigate whether there were strong correlations between the spectral bands used as predictors in some PLSR models and also between the grassland variables used as predictors in other PLSR models using the data sets used for each of the main chapters in this thesis. Figure 4.1 presents correlation matrices which used the smallest sample size as an example, where the correlations were found using data from Parsonage grasslands collected during the summer only (30 quadrats, data set used in Chapter 6). The correlation plots presented in Appendix Figures 1 and 2 used data collected during summer from seven grasslands across two locations (70 quadrats, data set used in Chapter 4) and from Parsonage grasslands collected across three seasons (90 quadrats, data set used in Chapter 5).

Figure 4.1a shows results from using CROPSCAN data while Figure 4.1b shows results from using Rikola camera (UAV) data. Correlation matrices were not produced for the ASD/SVC spectral devices as these devices have bands that match the CROPSCAN and Rikola camera. Figure 4.1c shows results from using mass data while Figure 4.1d shows results from using % cover data. The correlation matrix for the spectral bands indicated statistically significant correlations of $r < -0.8$ and $r > +0.8$ between bands in the visible part of the spectrum and also between some bands in the NIR region of the spectrum (Figure 4.1a and b). The correlation matrices for the mass and % cover-based grassland variables similarly resulted in a few significant *r* values $r < -0.8$ and $r > +0.8$ (Figure 4.1c and d). Furthermore, the p-value was calculated for each correlation and any correlation that was not considered to be significantly different from $r = 0$ (95% value) was greyed out. Similar results were produced from using CROPSCAN, mass and % cover data collected on all seven grasslands during summer (Appendix Figure 1) and on Parsonage grasslands collected over three seasons (Appendix Figure 2).

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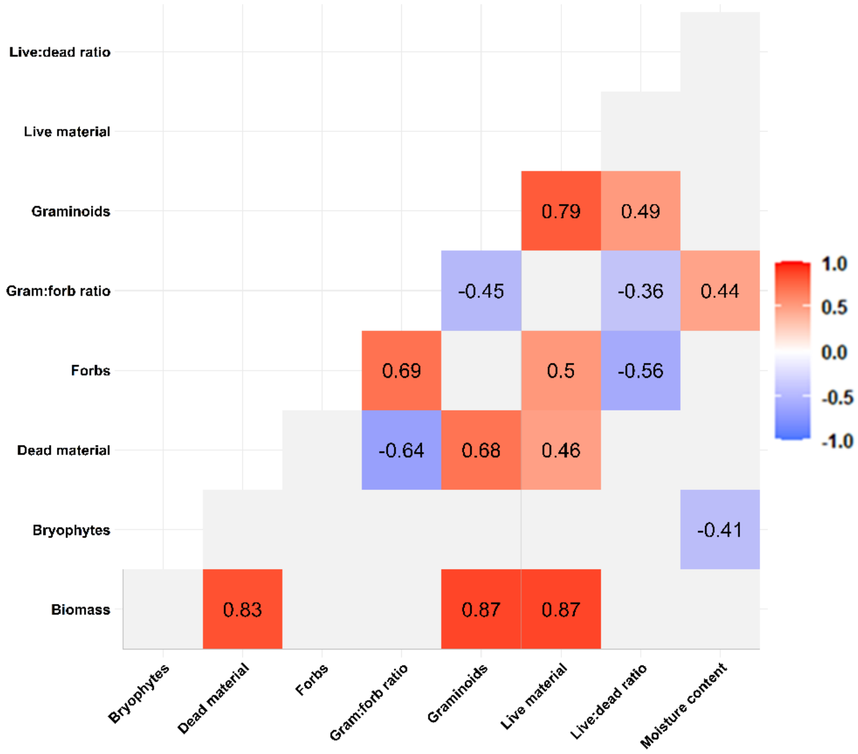


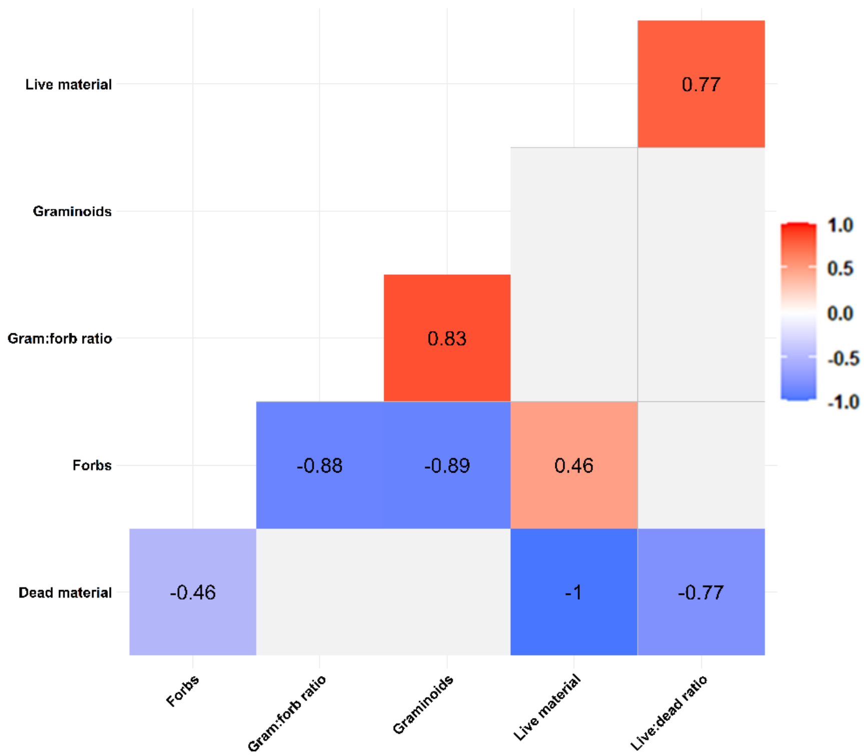




*Figure 4.1: Correlation matrices between predictors used in PLSR modelling a) spectral bands from CROPSCAN, b) spectral bands from Rikola VNIR camera, c) mass data, d) % cover data where n = 30 (data from Parsonage grasslands). Correlation coefficients that are not statistically significant (alpha >= 0.05) are blanked out.*

## 4.2. Grassland site characteristics

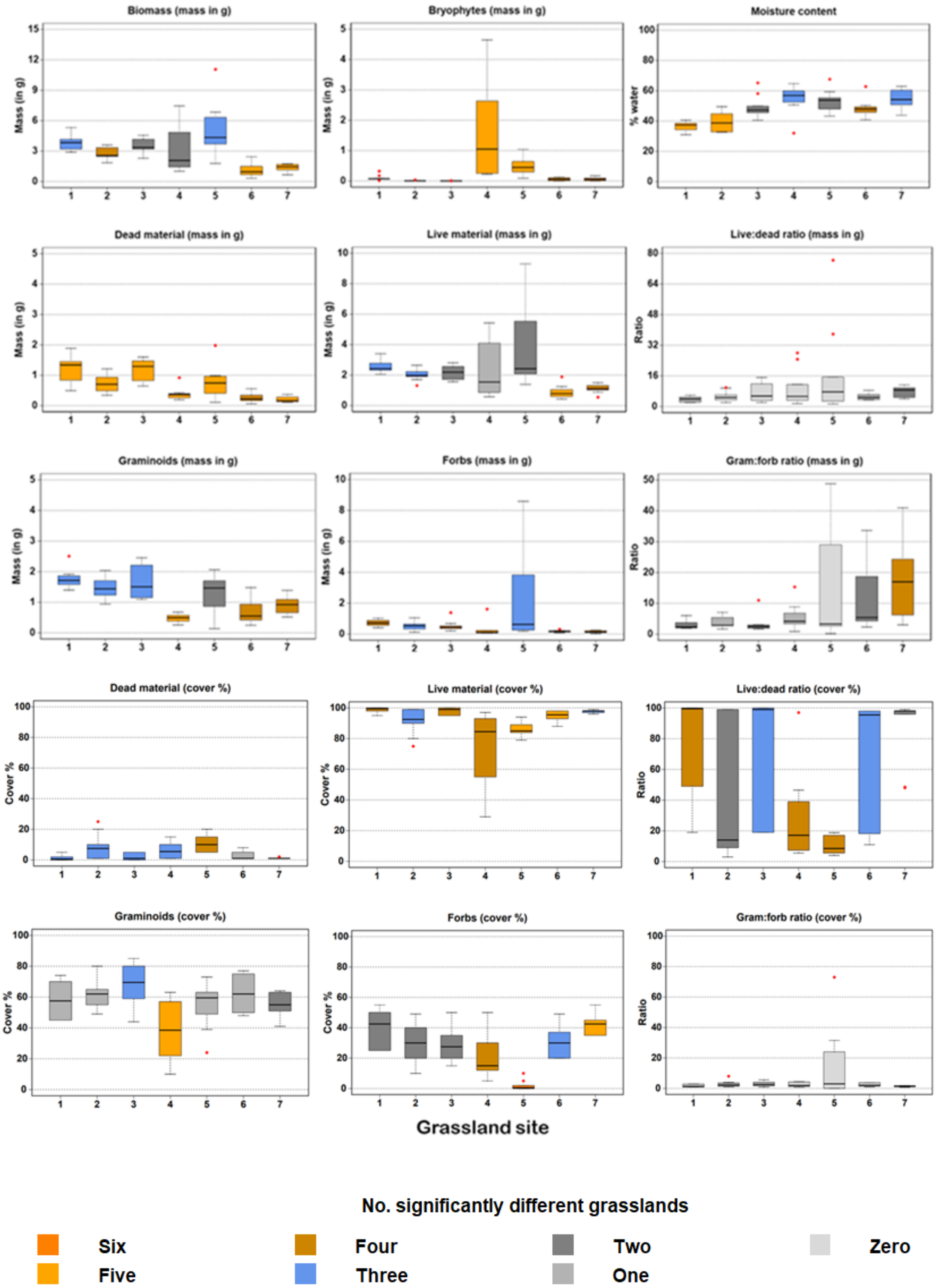


*Figure 4.2: Boxplots of grassland variables (mass in g and cover in %) for the seven grassland sites. The boxplot colours summarise the unpaired two-sample Wilcoxon test results between grassland types: A grassland variable was considered significantly different between two grasslands if $p<0.05$; the boxplot of each grassland site is coloured according to the number of sites from which it is significantly different.*

The Wilcoxon tests for the mass-based grassland variables show that for bryophytes mass, dead material mass and forbs mass; at least five of the seven grassland sites were significantly different in their distribution from at least four other sites. Three grassland sites were significantly different from at least four other sites for the grassland variables biomass, graminoids mass and moisture content. Live material mass, gram:forb ratio mass and live:dead ratio mass have less than three grasslands that were significantly different from at least four of the other grasslands.

The Wilcoxon tests for the % cover-based grassland variables show that all grassland sites were significantly different in their distribution from at least four other sites for dead material cover and live:dead ratio cover. Three grassland sites were significantly different from at least four other sites for forbs cover and live material cover. Gram:forb ratio cover and graminoids cover had no grasslands that were significantly different to at least four other grasslands.

Figure 4.3 shows the condition scores according to the CSM guidance at quadrat level for each grassland site, indicating the level of variation in condition within each site. Three sites (Sites 3, 4 and 5) show quadrat level conditions that range from bad to good; two other sites (Sites 2 and 7) have quadrat conditions that vary between bad and intermediate, and the two remaining sites (Sites 1 and 6) show all quadrats in good condition.

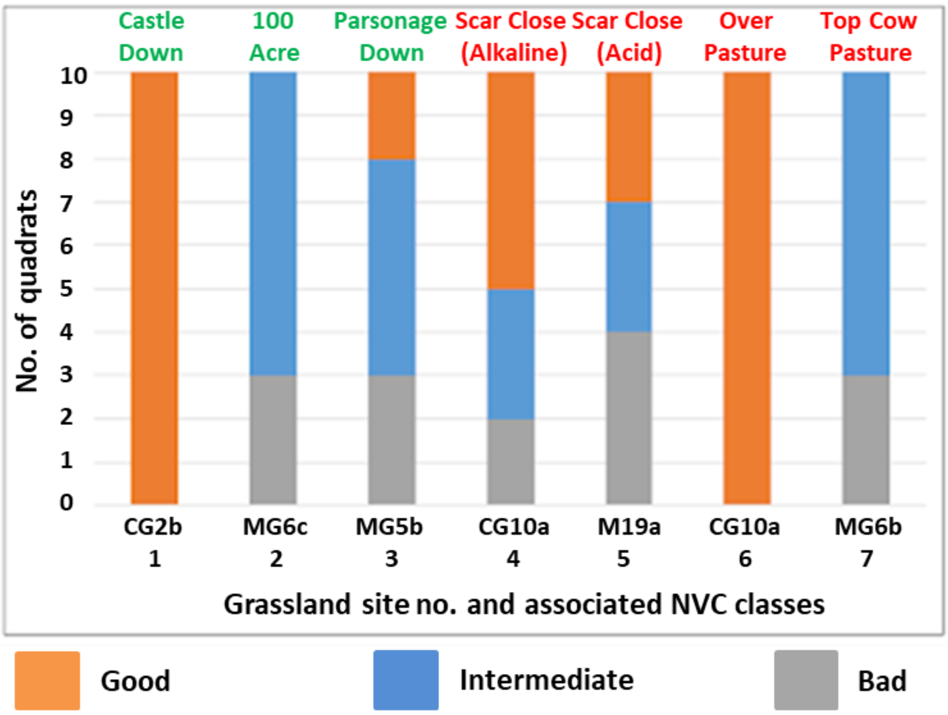



*Figure 4.3: Absolute numbers of quadrats of each level of condition per grassland according to the UKCSM criteria and grassland NVC classifications for each of the seven grassland sites. Sites 1 to 3 are for Parsonage Down NNR (names in green) and Sites 4 to 7 are for Ingleborough NNR (names in red). Good condition means that >80% UKCSM criteria are met, intermediate is 60-80% of criteria met and bad is <60% criteria met.*

## 4.3. Predicting grassland variables and condition using PLSR

The median $R^2$ and nRMSE results of using PLSR modelling where $R^2$ => 0.5 and nRMSE <= 100, from 45 runs for individual grasslands or 1000 runs for collective grasslands, to predict mass and % cover grassland variables plus CSM-condition using spectral data can be seen in Figure 4.4 while the full results are presented in Appendix Figure 3. The success in predicting these variables from spectral data is partly dependent on whether the models are using data from both locations (total of 70 quadrats), a single location (total of 30 or 40 quadrats which has been termed “collective analysis” for the three or four sites, respectively) or a single site (10 quadrats) with a broad trend of model performances improving (higher $R^2$ and lower nRMSE) when the data used is limited to a specific location and then site. Using the full band set (16 bands) including SWIR (i.e. FULL) or the VNIR only bands (14 bands), impacts only when the data used is limited to a specific grassland site.

When mass grassland variable data from all seven grasslands are analysed as one using data for both locations combined (given as top left plot in Figure 4.4a) the PLSR models for bryophytes mass, dead material mass and graminoids mass stand out with $R^2$ values of >0.5 and nRMSE <100. When % cover grassland variable data is used (given as top left plot in Figure 4.4c), only forbs cover has a $R^2$ value of >0.5 value and nRMSE value <100.

***Figure 4.4a - Parsonage (mass in g)***

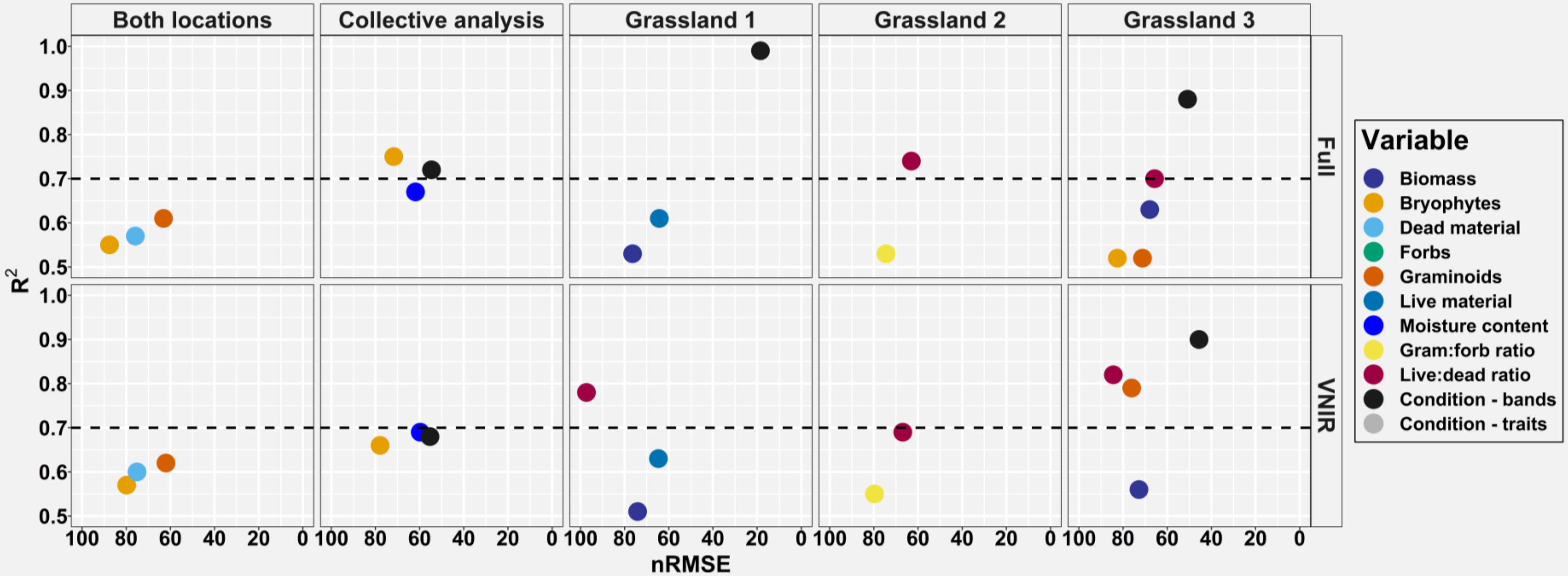


*Figure 4.4b - Ingleborough (mass in g)*

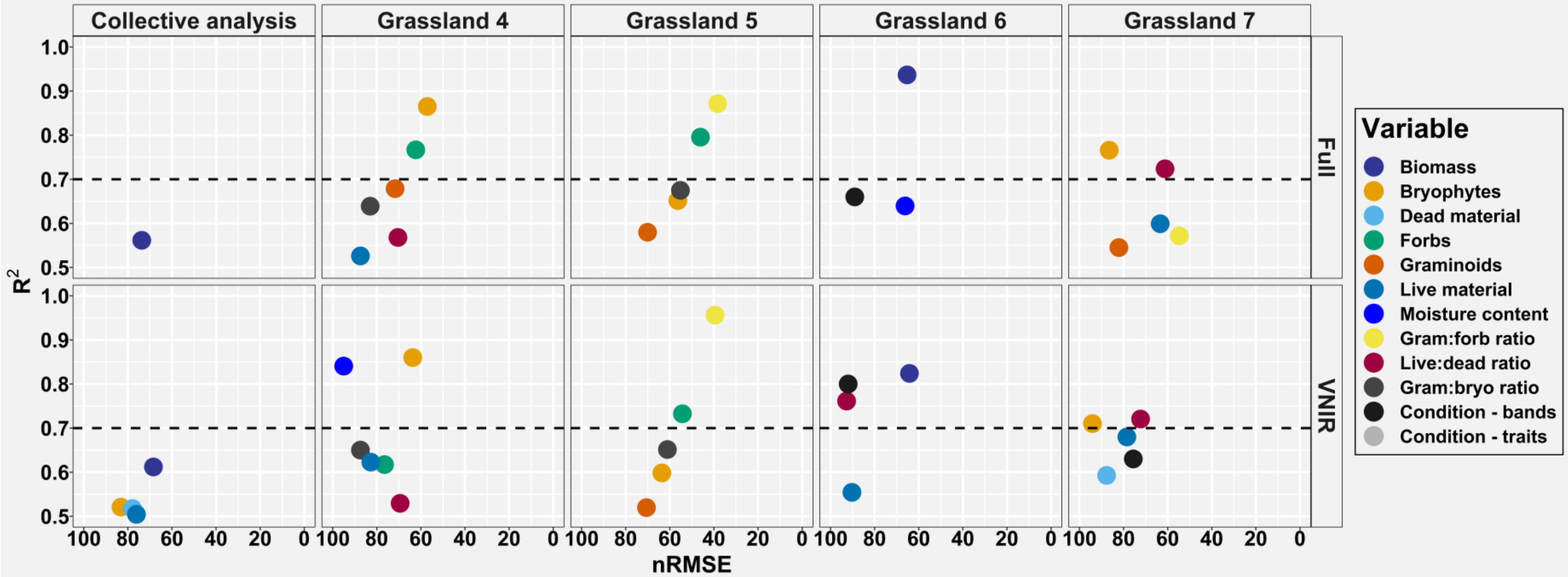
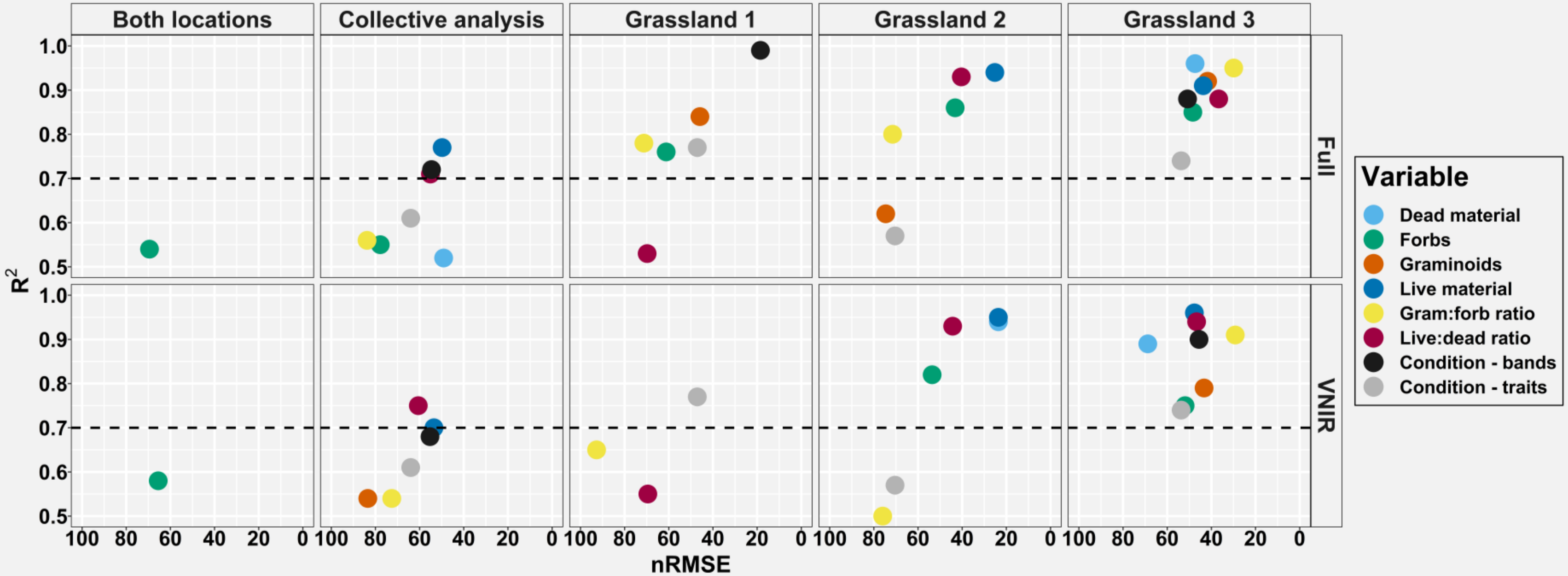


***Figure 4.4c - Parsonage (% cover)***



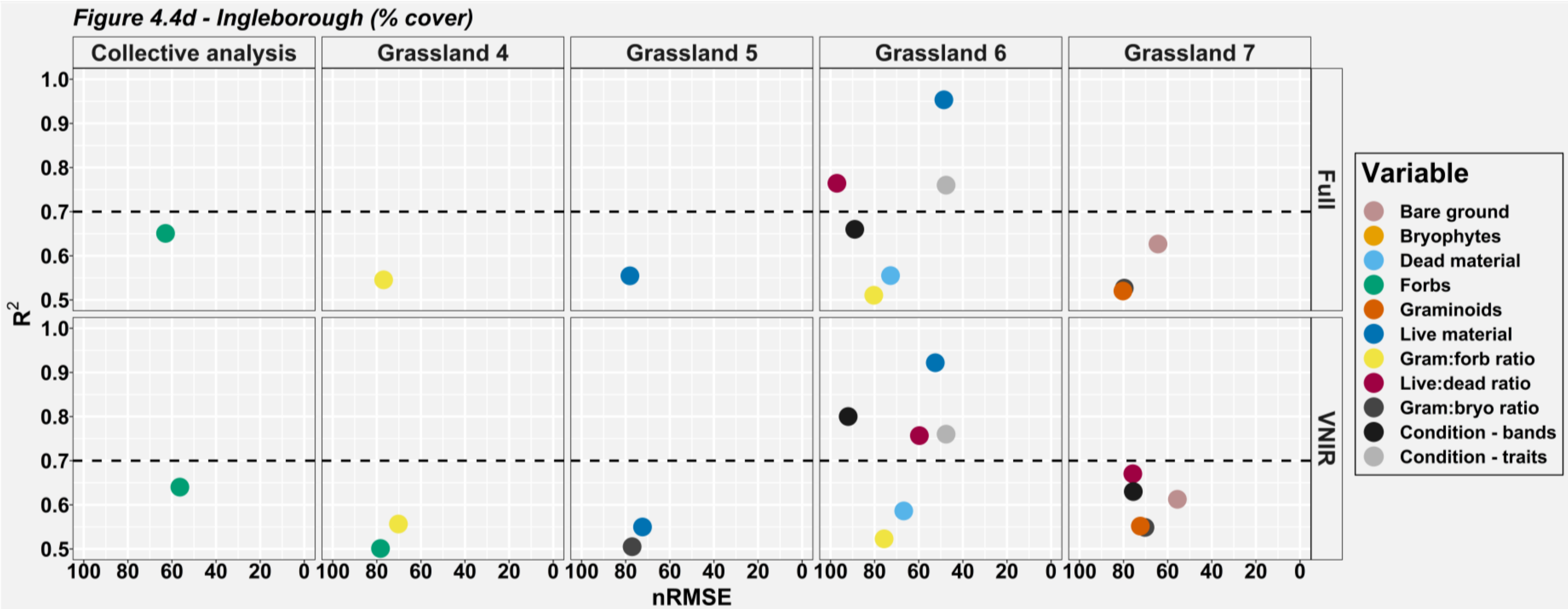



*Figure 4.4: Plots for results of 426 PLSR regressions where $R^2$ =>0.5 and nRMSE <=100, each of which represent the median* $R^2$ *and nRMSE values of the iterated model runs, where (i) spectral data (either FULL or VNIR) were used to predict grassland variables (coloured dots) and CSM based condition (black dot) and (ii) grassland variables were used to predict CSM based condition (white dot). Panels a and b show results for mass based analysis; c and d for % cover based analysis.*

When grassland sites from both locations are analysed collectively (all seven grasslands); bryophytes mass, dead material mass, graminoids mass and forbs cover were predicted with $R^2$ >0.5 and nRMSE <100 whilst other PLSR model runs produced $R^2$ values <0.5. When grassland sites from each location are analysed collectively (referring to three and four sites combined for Parsonage and Ingleborough, respectively), most grassland variables were predicted with $R^2$ >0.5 and nRMSE <100 for Parsonage when predicting % cover data, whereas only a few variables achieved this level of accuracy when predicting mass data; bryophytes mass and moisture content plus CSM-condition (black dots in Figure 4.4) when predicting with spectra. Relatively few variables were predicted with $R^2$ >0.5 and nRMSE <100 for Ingleborough; only forbs cover, biomass and dead material mass.

When grassland sites at Parsonage or Ingleborough are analysed individually for predicting mass or % cover grassland variable data, many PLSR model fits produced $R^2$ values >0.5 and nRMSE <100 except for Grasslands 2 and 3 when using mass grassland variable data or Grassland 5 when using % cover grassland variable data where only 2-3 model fits produced $R^2$ values >0.5 and nRMSE <100.

Of 426 model runs in total (using mass and % cover data); 188 produced results of $R^2$ >0.5 and nRMSE <100; with live:dead ratio (27 model runs) producing the most followed by forbs, graminoids, dead material, gram:forb ratio (19-21 model runs for each grassland variable). More accurate performances in order of number of $R^2$ >0.7 results are for live:dead ratio (17 model runs), forbs (12 model runs), live material (11 model runs) and gram:forb ratio (10 model runs).

The success in predicting grassland variables from spectral data was dependent on whether the variables were expressed in terms of mass or % cover and the difference in performance varied from small to substantial depending on the grassland variable. When 144 comparable mass and % cover based models are compared against each other; % cover achieved higher $R^2$ results than mass for Parsonage and Ingleborough locations in 9 of 14 comparable models and lower nRMSE results in 10 of 14 comparable models. Also, % cover achieved higher $R^2$ results than mass for Parsonage in 44 of 54 comparable models and lower nRMSE results in 42 of 54 comparable models. For Ingleborough grasslands, mass had higher $R^2$ results than % cover for 43 of 76 comparable models and lower nRMSE results in 49 of 76 comparable models.

The impact of utilising FULL spectral bands (16 bands across 470-1640nm range) as predictors relative to just the VNIR bands (14 bands across 470-870nm range) appears to be site specific, but generally, the difference in model performance is small ($R^2$ <0.05 and nRMSE <10). Of 188 model runs that produced results of $R^2$ >0.5 and nRMSE <100, 94 of them used FULL spectrum data whilst 86 of them used VNIR spectral data, where the other 8 models predicted CSM-condition with grassland variables and therefore did not utilise spectral data.

When the $R^2$ and nRMSE results of 140 comparable models were compared between models that used FULL spectral data as predictors and models that used VNIR spectral data as predictors, VNIR produced stronger $R^2$ results in 10 of 14 model runs and lower nRMSE results for 12 of 14 model runs when comparing results from analysing both locations. FULL produced stronger $R^2$ results and lower nRMSE results in 40 of 48 model runs when comparing results from analysing Parsonage grasslands. VNIR produced stronger $R^2$ results in 44 of 78 model runs and lower nRMSE results for 37 of 78 model runs when comparing results from analysing Ingleborough grasslands.

The PLSR models that used spectral data to predict CSM-condition delivered results of $R^2$ >0.5 (mostly $R^2$ =>0.65) and nRMSE <100 when grasslands were analysed collectively and for Grassland 3 (Figure 4.4). When grassland variables were used to predict CSM-condition, models based on % cover data from individual sites or from Parsonage grasslands collectively performed best, most achieving $R^2$ >0.5 and nRMSE <100.

## 4.4. Stability and consistency between model runs using the same response variable

Figure 4.5 shows the % coefficient of variation (CV) found from the iterated model runs for the resulting $R^2$ and nRMSE values of the site specific PLSR models that were calculated to evaluate the stability of model performances across sites for specific grassland variables. These results suggest that the performance of the models for bryophytes cover, forbs cover and live:dead ratio cover are relatively stable. Most grassland variables have a similar level of consistency when mass data are used. Overall, mass based models produce more consistent nRMSE results across sites compared to % cover based models and VNIR-based models have slightly more consistent nRMSE results between sites than FULL-based models. There is no overall trend showing which sets of results have more consistent $R^2$ results and whether using mass/cover or FULL/VNIR for more consistent results is grassland variable specific.

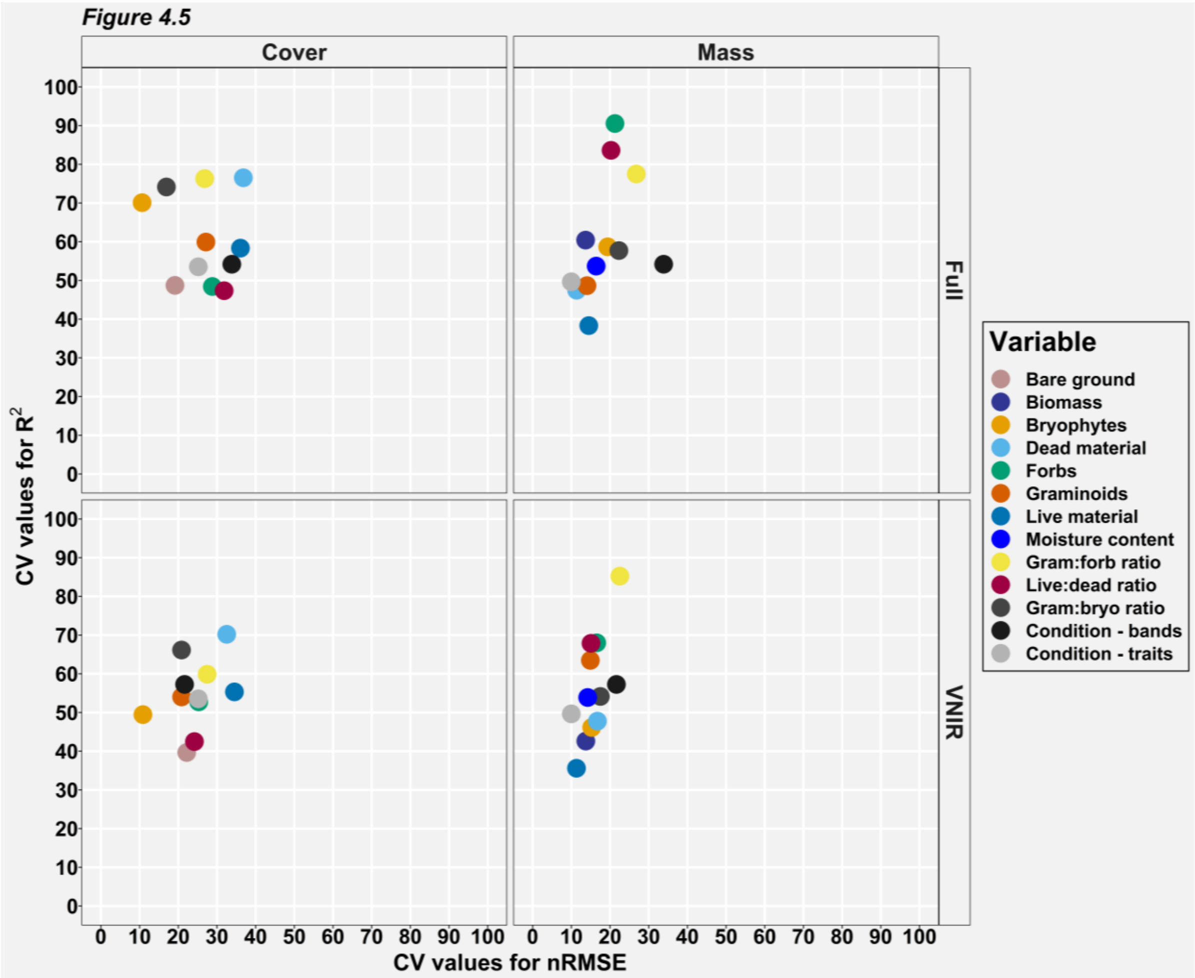



*Figure 4.5: % coefficient of variation (CV) plots for the $R^2$ and nRMSE results of the site specific PLSR models grouped per treatment (% cover - left; mass - right) and spectral input data (full spectrum - top; VNIR - bottom).*

## 4.5. VIP analysis for spectral band and grassland variable selection

Figure 4.6 shows the results of using a VIP analysis to understand which spectral bands were the most important predictors for predicting grassland variables, where only results =>

1 have been included and therefore most of the results are not shown here. The results suggest that the two SWIR bands (1240 and 1640nm) are the most important for predicting grassland variables and condition across all grasslands, along with the red edge (647nm) and upper NIR bands for some grasslands. When VNIR data are used; the upper NIR bands plus the red edge are most important for predicting grassland variables and CSM-condition. When grassland variables are used to predict condition (Figure 4.7); gram:bryo ratio cover (where applicable), gram:forb ratio cover and live:dead ratio cover plus forbs cover and graminoids cover are important for a range of grasslands. Other grassland variables were only important in predicting CSM-condition on some grasslands, with these grasslands being different depending on the grassland variable.

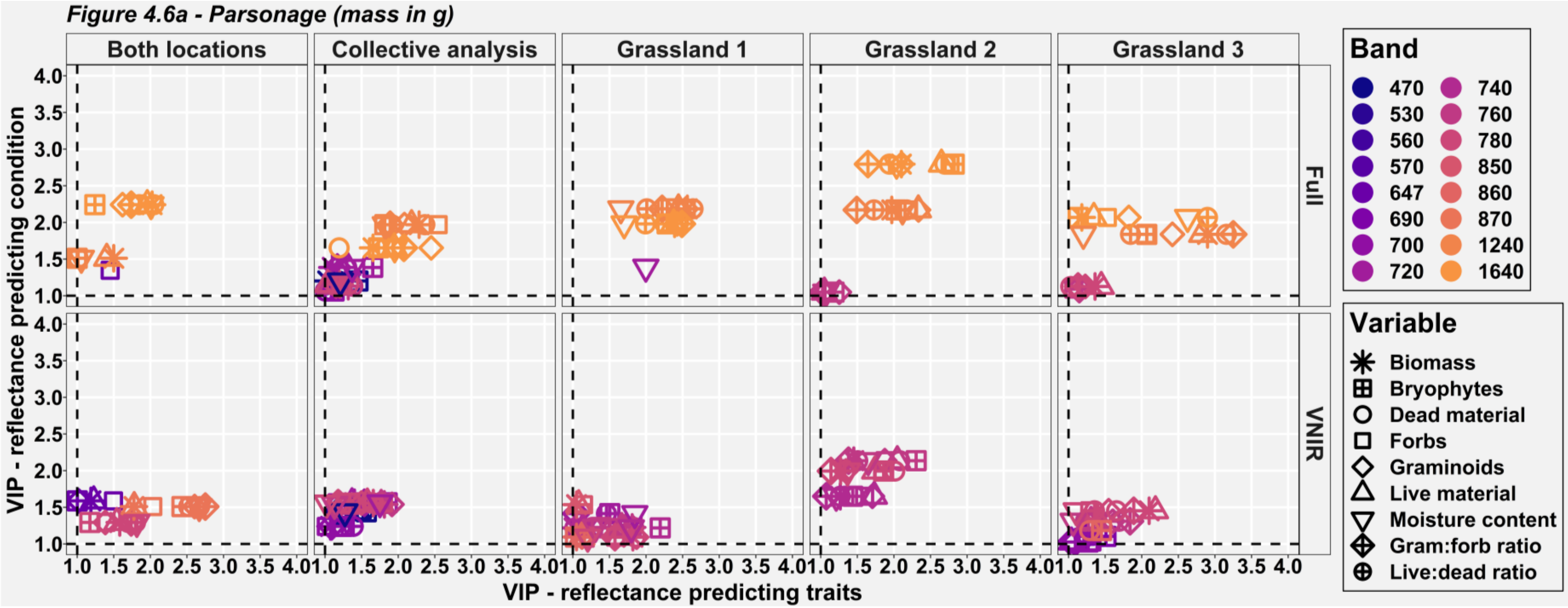


Figure 4.6a - Parsonage (mass in g)
Both locations
Collective analysis
Grassland 1
Grassland 2
Grassland 3
Full
VNIR
VIP - reflectance predicting condition
VIP - reflectance predicting traits
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Band
470
530
560
570
647
690
700
720
740
760
780
850
860
870
1240
1640
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio

2555

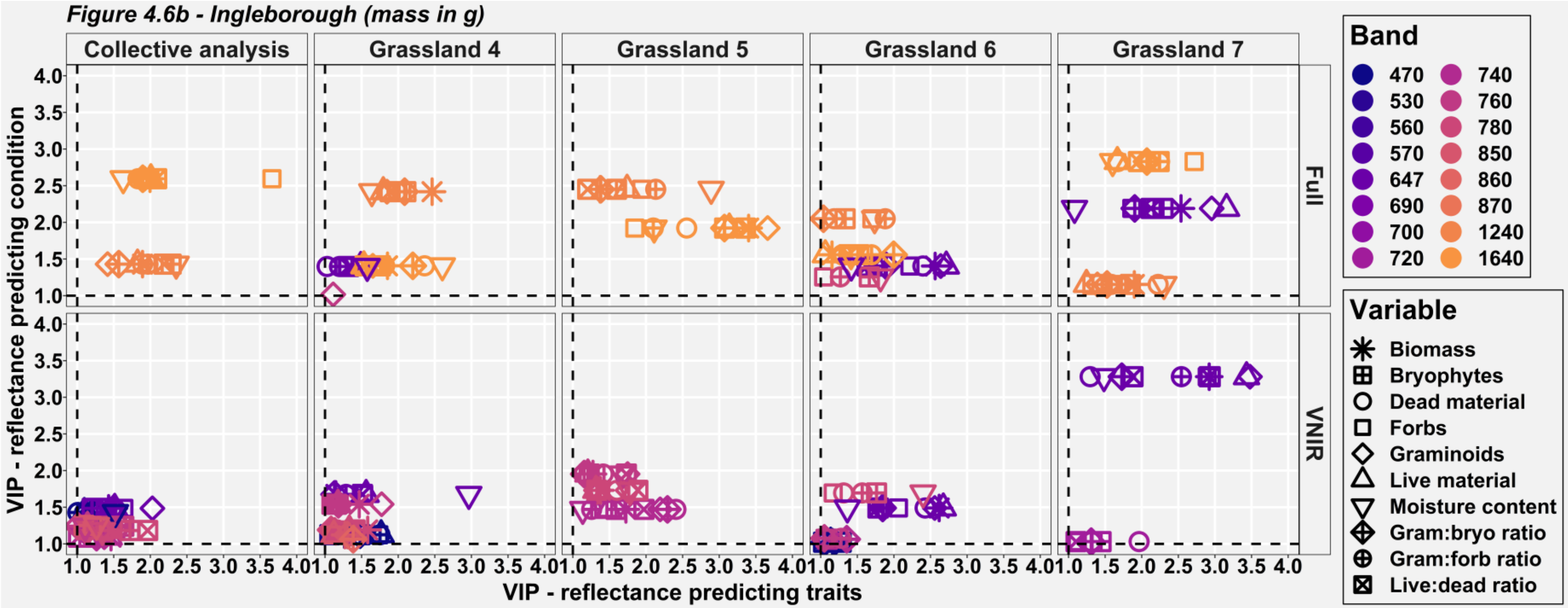
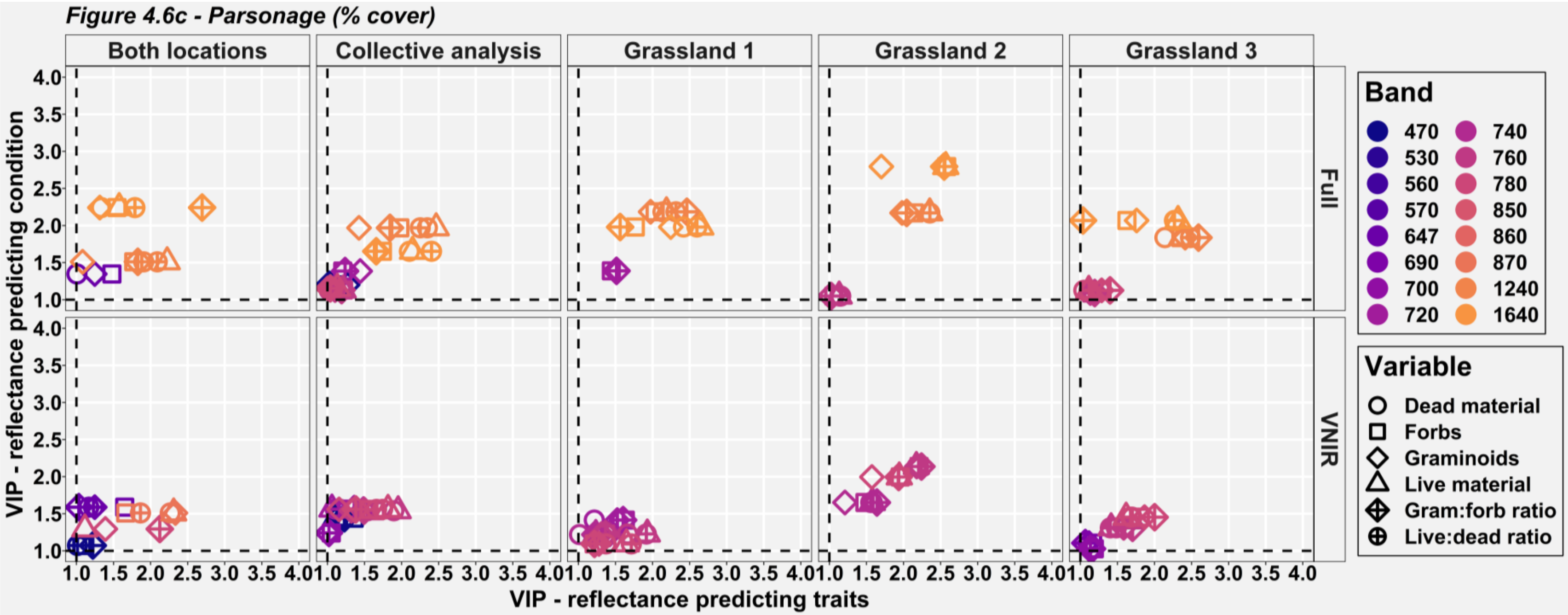


Figure 4.6b - Ingleborough (mass in g)
Collective analysis
Grassland 4
Grassland 5
Grassland 6
Grassland 7
Full
VNIR
VIP - reflectance predicting condition
VIP - reflectance predicting traits
Band
470
530
560
570
647
690
700
720
740
760
780
850
860
870
1240
1640
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:bryo ratio
Gram:forb ratio
Live:dead ratio

2556

2557 
Figure 4.6c - Parsonage (% cover)
Both locations
Collective analysis
Grassland 1
Grassland 2
Grassland 3
Full
VNIR
VIP - reflectance predicting condition
VIP - reflectance predicting traits
1.0 1.5 2.0 2.5 3.0 3.5 4.0
Band
470 530 560 570 647 690 700 720 740 760 780 850 860 870 1240 1640
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio

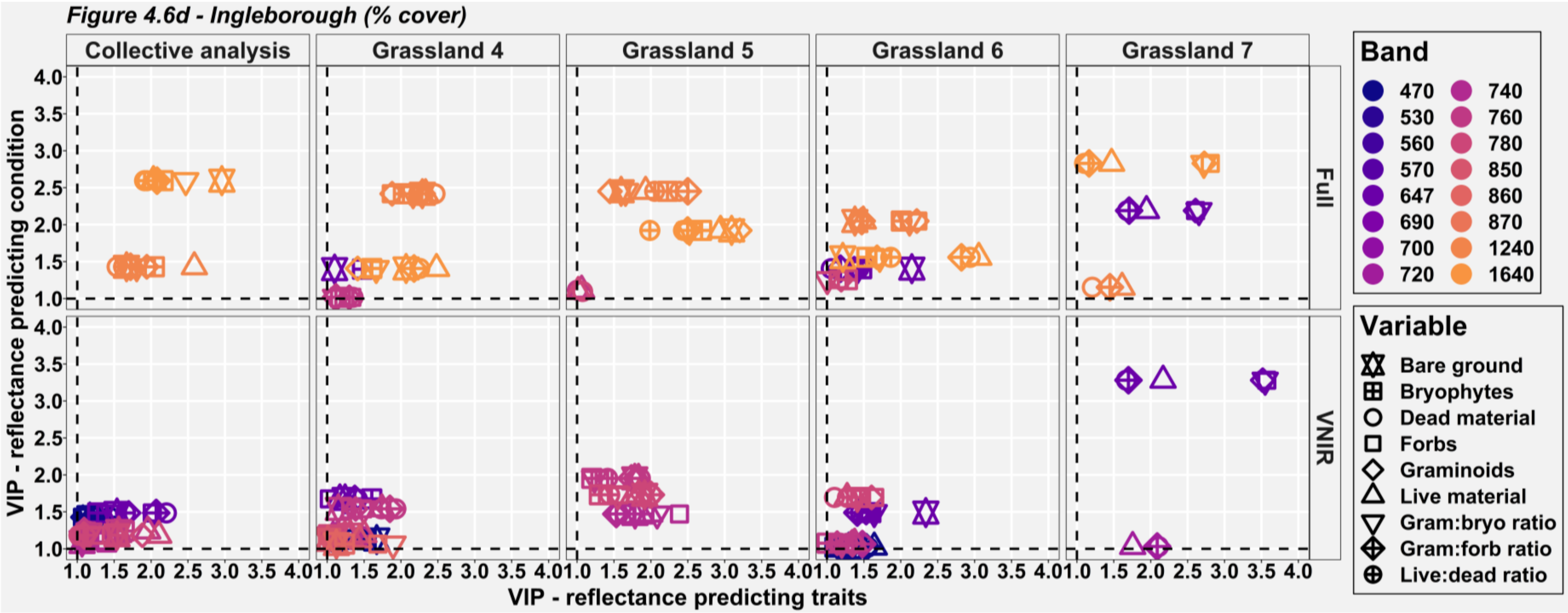



*Figure 4.6: VIP plots showing which combinations of spectral bands (predictors) and which responses (grassland variables on x axis and CSM-condition on y axis) are most important in the PLSR models used in this study.*

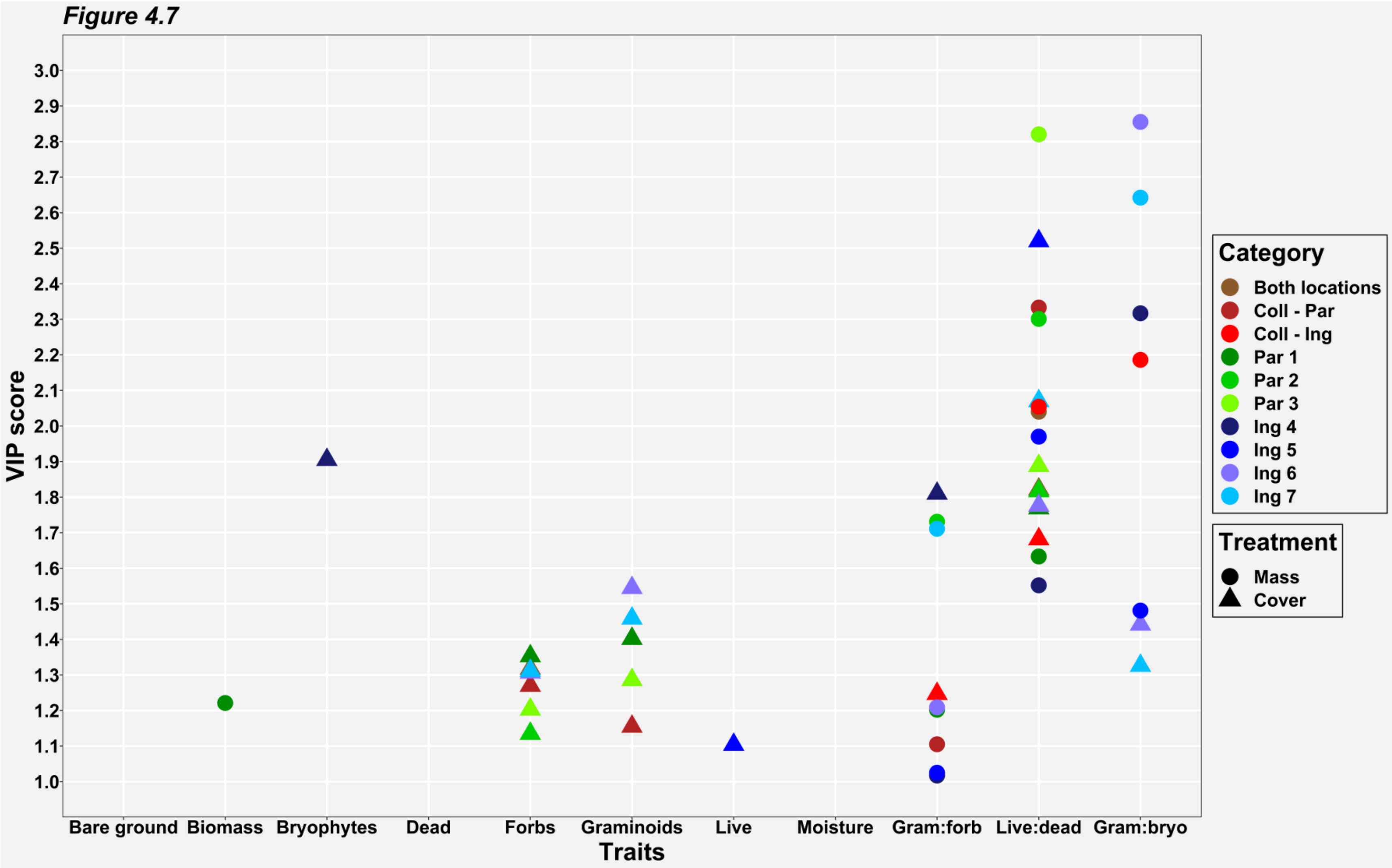


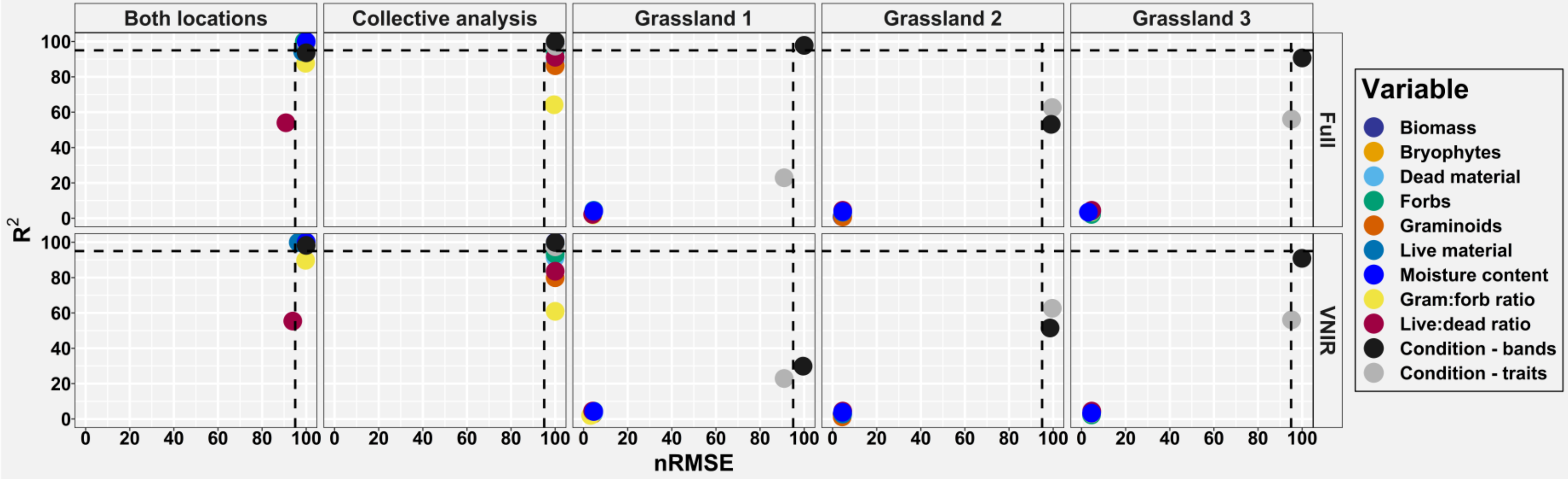

*Figure 4.7: VIP plot showing which grassland variables are most important in predicting CSM-condition using either mass or % cover data from analysing grasslands individually or collectively for one or both locations.*

## 4.6. Comparison of PLSR models trained with actual data and PLSR models trained with random data

The actual data results, as seen in Figure 4.4, were compared against the results of iterative model runs (either 44 for individual grassland analysis or 999 for collective grassland analysis) with randomised response variable values to test if the results run with the actual data genuinely produce reasonable results in comparison to models with randomised data. The results are plotted in Figure 4.8, where points close to the top right corner of the graph are of interest.

The results suggest that models using the true data (actual models) are only superior to models using randomised data (random models) depending on the size and combination of the data being used. At the 95% level, actual models consistently perform more accurately than random models when data from both locations are used. When using data from collective analysis (30 quadrats for Parsonage and 40 for Ingleborough) the actual models almost always produce stronger nRMSE results but not stronger $R^2$ results. Using data from individual grasslands (10 quadrats) to train PLSR models results in models that are not considered to be more reliable than a random model.

*Figure 4.8a - Parsonage (mass in g)*



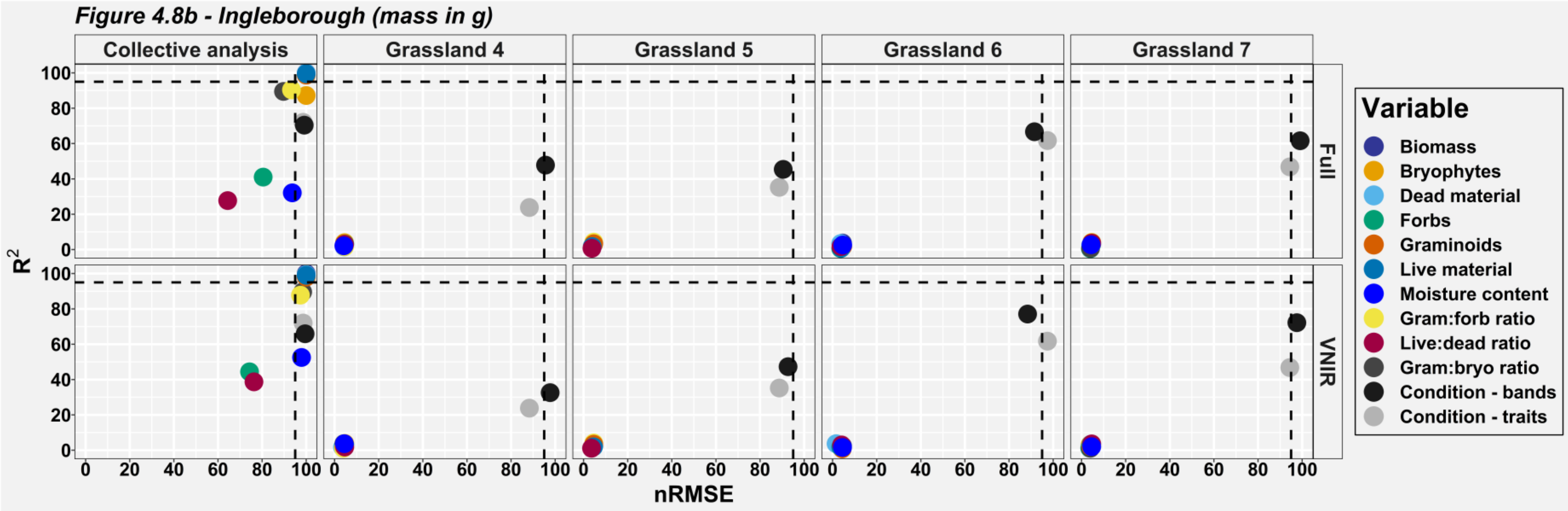
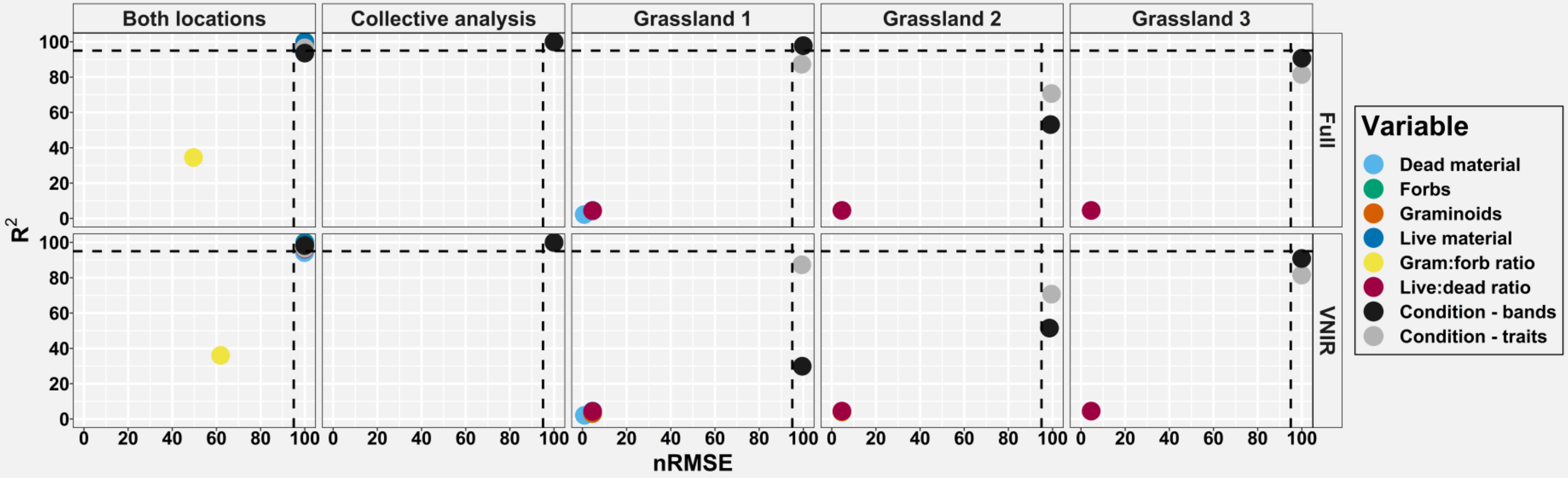


Figure 4.8b - Ingleborough (mass in g)
Collective analysis
Grassland 4
Grassland 5
Grassland 6
Grassland 7
Full
VNIR
R2
nRMSE
0
20
40
60
80
100
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Gram:bryo ratio
Condition - bands
Condition - traits

2583

*Figure 4.8c - Parsonage (% cover)*



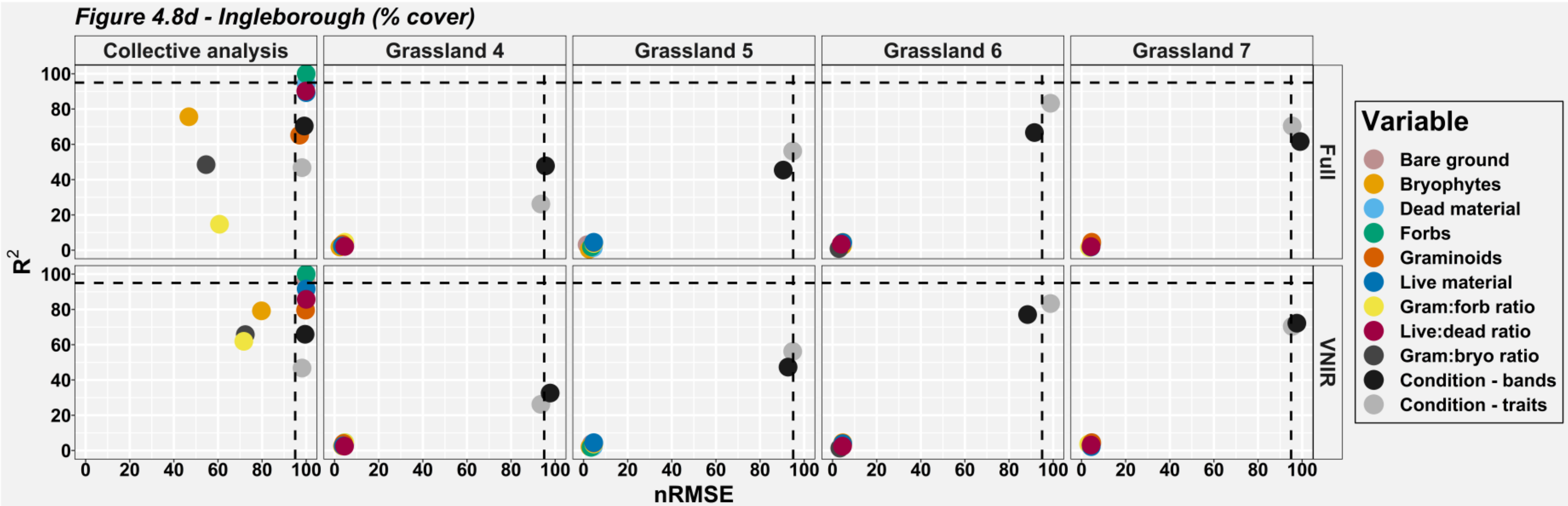


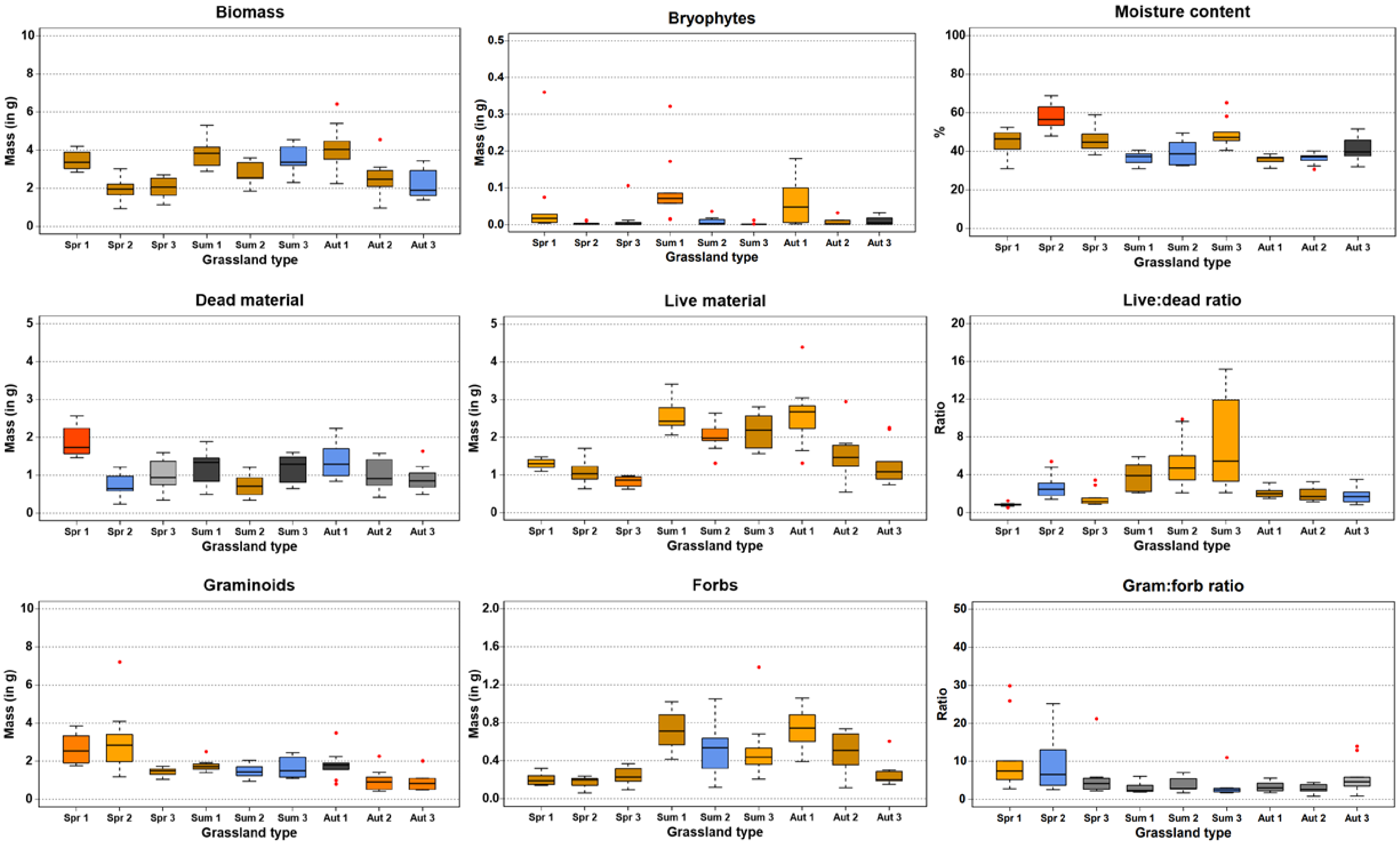

*Figure 4.8: Comparison of the median values of iterated model runs using actual response data and 44 or 999 model runs (dependent on whether grasslands were analysed individually or collectively) using randomised response data. The plot shows the ranking of the actual model out of the maximum iterated runs (either 45 for individual grasslands or 1000 for collective grasslands), where high rankings (e.g. >950 for the 95% level) are sough*

# Chapter 5 - Assessing seasonal effects on the condition of calcareous semi-natural grasslands using CROPSCAN field radiometry at patch level (1m$^2$)

## 5.1. Grassland site characteristics

The boxplots seen in Figure 5.1 show the quantity of each variable for each grassland and season, including the results of significant difference tests between grassland types across seasons. Overall, the Wilcoxon tests for grassland variables show that some mass-based grassland variables are generally significantly different on the three different grasslands across three seasons whilst cover-based grassland variables were generally not significantly different to each other. The Wilcoxon tests for the mass-based variables show that for variables biomass, bryophytes mass, live material mass, live:dead ratio mass and forbs mass most of the nine grassland site and season combinations were significantly different in their distribution from at least five other site-season combinations. The Wilcoxon tests for the cover-based grassland variables shows that live:dead ratio cover was generally significantly different in distribution between grasslands and seasons. Also, at least two grasslands during spring had significantly different distributions for the variables dead material cover, live material cover and graminoids cover when compared to other site-season combinations but other grassland variables had no grasslands that were significantly different to at least four other site-season combinations.

2612


Biomass
Mass (in g)
Bryophytes
Mass (in g)
Moisture content
%
Dead material
Mass (in g)
Live material
Mass (in g)
Live:dead ratio
Ratio
Graminoids
Mass (in g)
Forbs
Mass (in g)
Gram:forb ratio
Ratio
Spr 1
Spr 2
Spr 3
Sum 1
Sum 2
Sum 3
Aut 1
Aut 2
Aut 3
Grassland type

2613

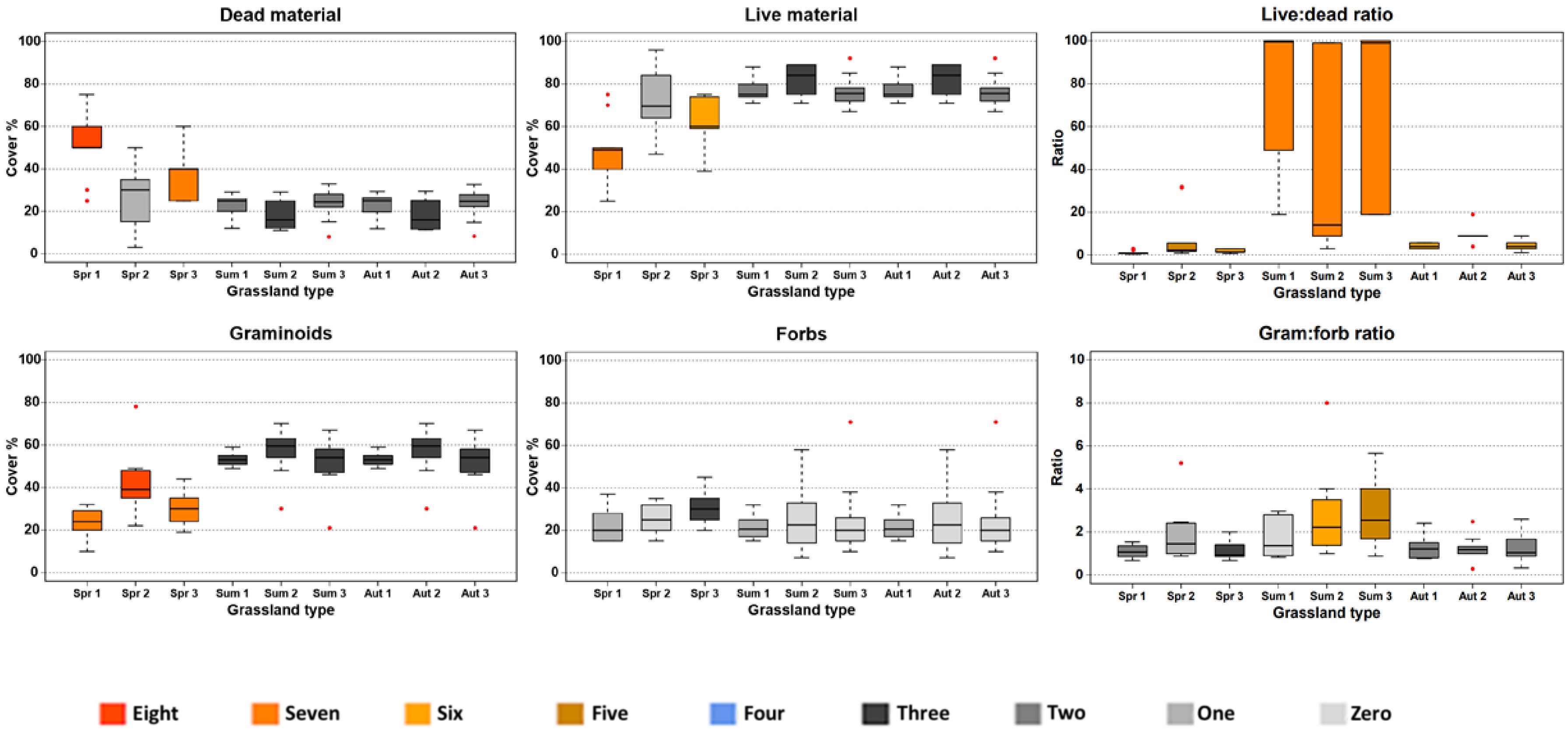



Figure 5.1: *Boxplots of the mass or % cover values of grassland variables for the three grassland sites. The boxplot colours summarise the unpaired two-sample Wilcoxon test results between grassland types and seasons: a grassland variable was considered significantly different between two grasslands if p<0.05; the boxplot of each grassland site is coloured according to the number of different site-season combinations from which it is significantly different.*

## 5.2. Predicting grassland variables and CSM-condition using PLSR

The median $R^2$ and nRMSE results of the PLSR modelling from the iterated model runs to predict mass and % cover grassland variables including CSM-condition variables can be seen in Figures 5.2 and 5.3 Overall, most variables were predicted with $R^2$ values >0.5 and nRMSE results <100 for at least some grasslands and seasons, but there are few patterns where a particular variable is predicted consistently across grasslands and seasons. Analysing data from all grasslands collectively (*n* = 30 or 90 for one or for all three seasons) produced PLSR models with $R^2$ >0.5 and nRMSE <100 for a similar number of grassland variables as analysing data from single sites (*n* = 10 or 30 for one or all three seasons) for most seasons, a clear exception being autumn for some grasslands when using % cover variable data. Removing the SWIR bands before analysis (14 bands, labelled VNIR) does not appear to have a big impact on the results relative to using the full spectral data set (16 bands, labelled FULL).

### 5.2.1. Mass-based grassland variable data

The results of using grassland variables derived from mass data as response data in the model runs where $R^2$ => 0.5 and nRMSE <= 100 can be seen in Figure 5.2 and the full results are presented in Appendix Figure 4. When grasslands are analysed collectively for all seasons (*n* = 90); graminoids mass (when using FULL), live material mass and live:dead ratio mass have $R^2$ values 0.5-0.7 but all other results are <0.5. For spring (*n* = 30); biomass, dead material mass, graminoids mass, live material mass and live:dead ratio mass all produced results of $R^2$ >0.5 and nRMSE results <100. For summer (*n* = 30); bryophytes, moisture content and CSM-condition predicted with spectral data produced results of $R^2$ =>0.5 and nRMSE results <100. For autumn (*n* = 30); biomass, forbs mass, graminoids mass, and live material mass had results of $R^2$ =>0.5 and nRMSE results <100.

When grasslands are analysed individually (n = 30 for all seasons or n = 10 for one season), there were some significant results but there is no obvious pattern in the results for any grassland variable except that gram:forb ratio mass is predicted consistently with $R^2$ values =>0.5 for Grassland 2. The grassland variables that produce the greatest number of significant results are biomass, graminoids mass and live material mass plus live:dead ratio mass when using VNIR.

Of 512 model runs (Figures 5.2 and 5.3); 243 produced $R^2$ results => 0.5 and nRMSE <100, 128 of which have $R^2$ results => 0.7. All grassland variables except bryophytes mass had >10 results of $R^2$ =>0.5 and nRMSE <100. Live material mass, graminoids mass and live:dead ratio mass have the most PLSR models with $R^2$ results => 0.5 and nRMSE <100 with 38, 39 and 40 respectively. Using % cover grassland variable data produced 119 PLSR models with $R^2$ results => 0.5 and nRMSE <100 whilst using mass grassland variable data produced 124 such results, suggesting that using mass grassland variables a similar number of moderate to strong PLSR models than using % cover data.

Analysing data from all grasslands collectively produced fewer PLSR models with $R^2$ results => 0.5 and nRMSE <100 (50) than analysing data from individual grasslands; 62 for Grasslands 1 and 2, and 70 for Grassland 3. A similar number of PLSR models with $R^2$ results => 0.5 and nRMSE <100 results were produced for FULL and VNIR; Using FULL spectral data produced 125 such results whilst using VNIR spectral data produced 118 such results. Using data from all seasons produced more PLSR models with $R^2$ results => 0.5 and nRMSE <100 (69) than using data from one season; 53, 57 and 63 for spring, autumn and summer respectively. The results for one season, particularly for spring, could have been affected by a relatively high quantity of dead material on the grasslands (Yang and Guo, 2014).

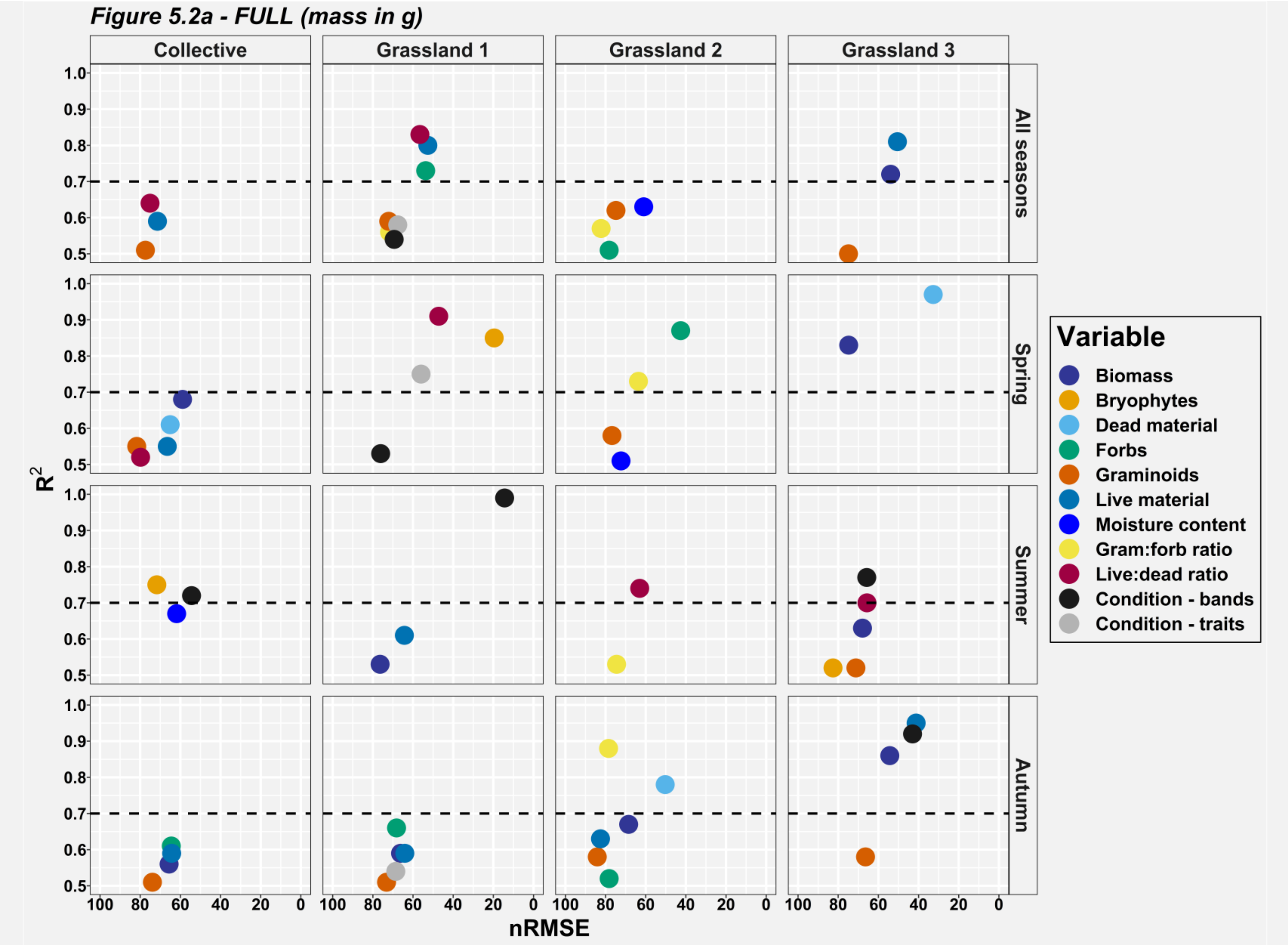


Figure 5.2a - FULL (mass in g)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

2674

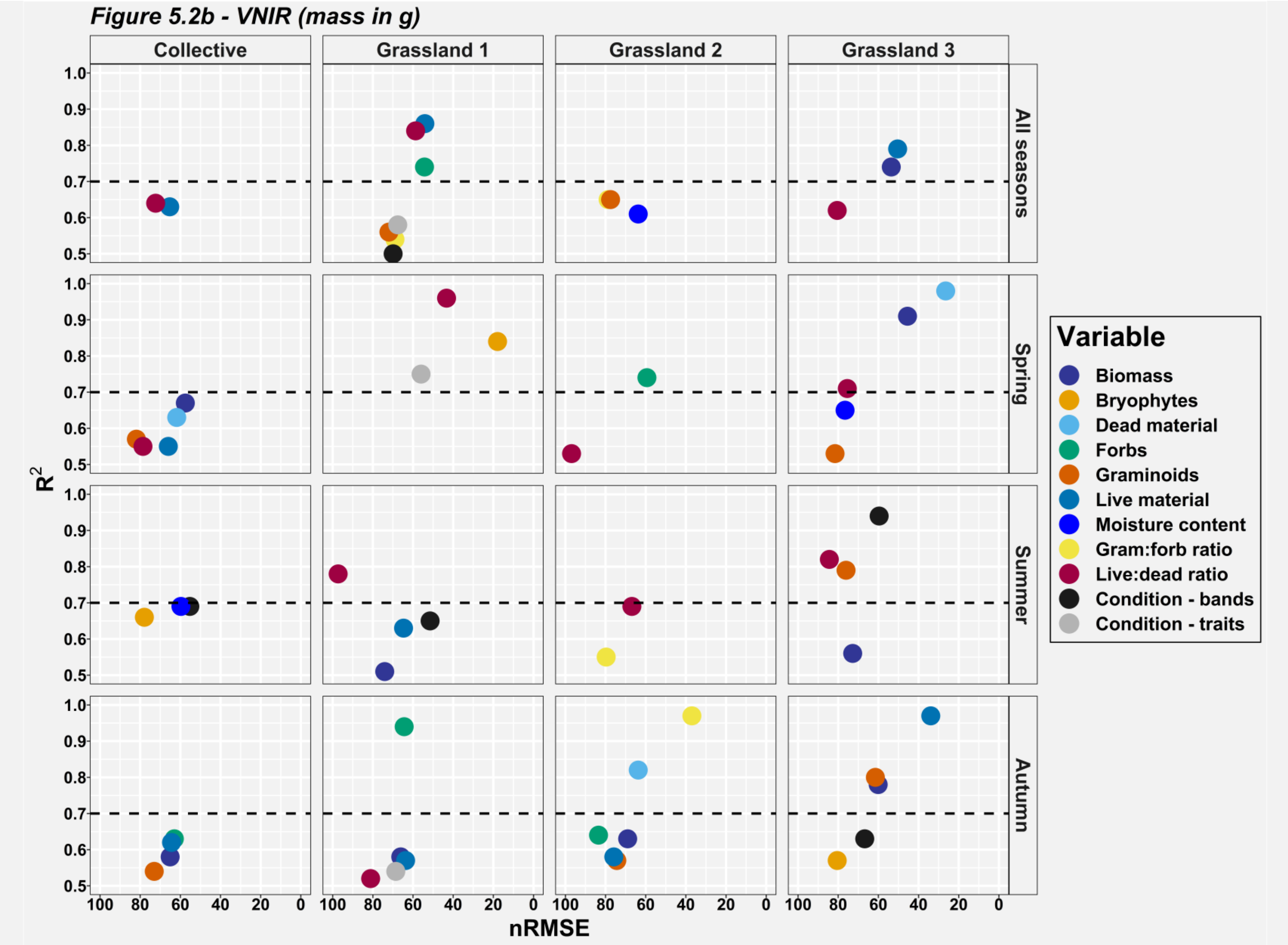


Figure 5.2b - VNIR (mass in g)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

2675

*Figure 5.2: Median results of iterated model runs where spectral data were used to predict CSM-condition and mass-based grassland variables for each of the three seasons (n = 10 or 30) and for all seasons (n = 30 or 90). Also included are the results of predicting CSM-condition using grassland variables as predictors.*

### 5.2.2. Cover-based grassland variable data

The results of using % cover grassland variable data as response data can be seen in Figure 5.3. When grasslands are analysed using data from all seasons; most grassland variables produced significant results for at least one grassland but dead material cover, graminoids cover, live material cover and live:dead ratio cover consistently produced $R^2$ values => 0.5 and nRMSE <100. When grasslands are analysed collectively for one season, most grassland variables were predicted with $R^2$ values => 0.5 for summer but almost all had $R^2$ values <0.5 except dead material cover and live:dead ratio cover when using VNIR data. When grasslands are analysed individually for one season, the grassland variables that produced significant results for all or nearly all of these grasslands and seasons (except Grasslands 1 and 2 for autumn) include forbs cover, graminoids cover, live material cover and live:dead ratio cover.

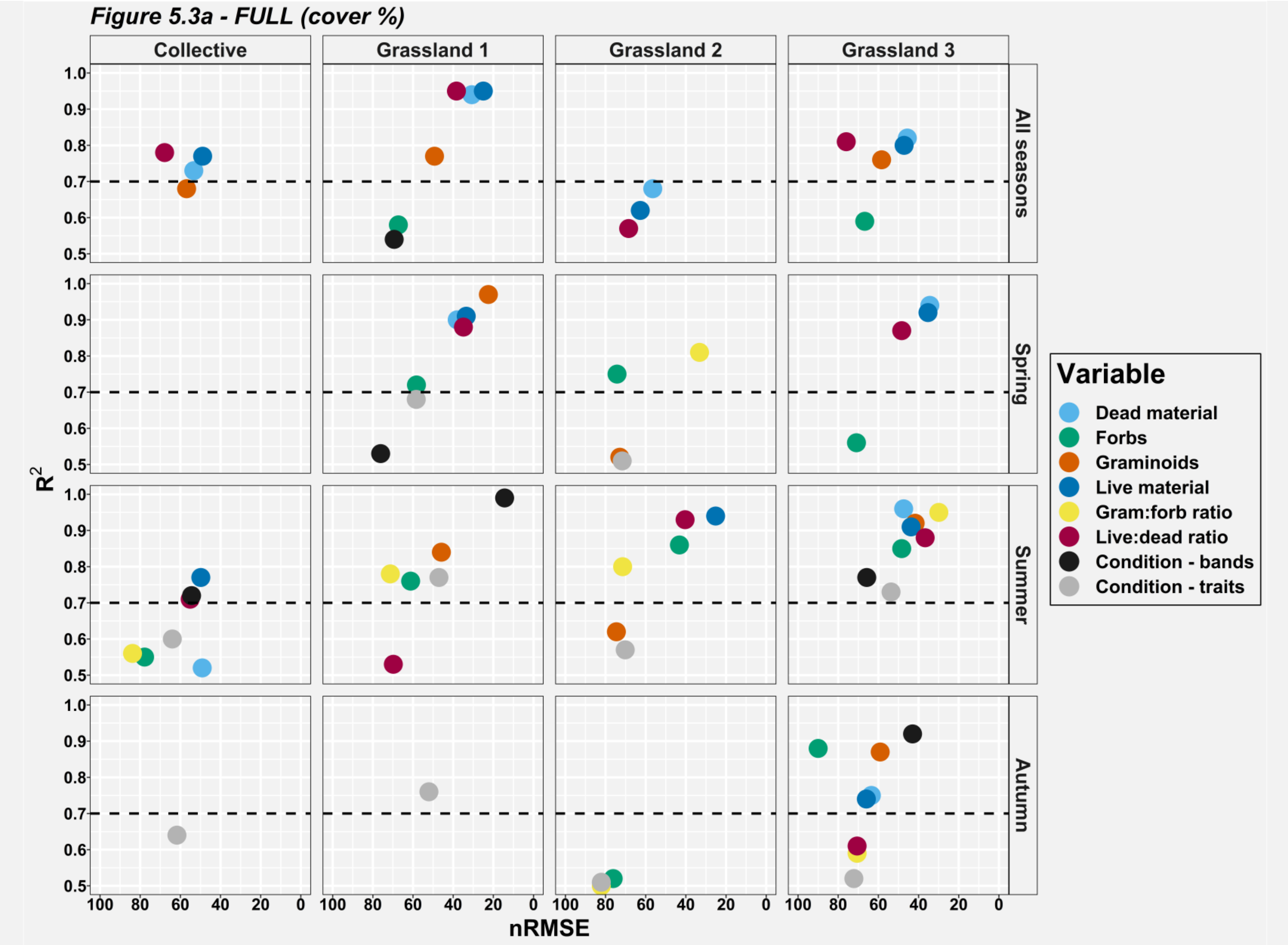


Figure 5.3a - FULL (cover %)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
1.0
0.9
0.8
0.7
0.6
0.5
100
80
60
40
20
0
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

2694

*Figure 5.3b - VNIR (cover %)*

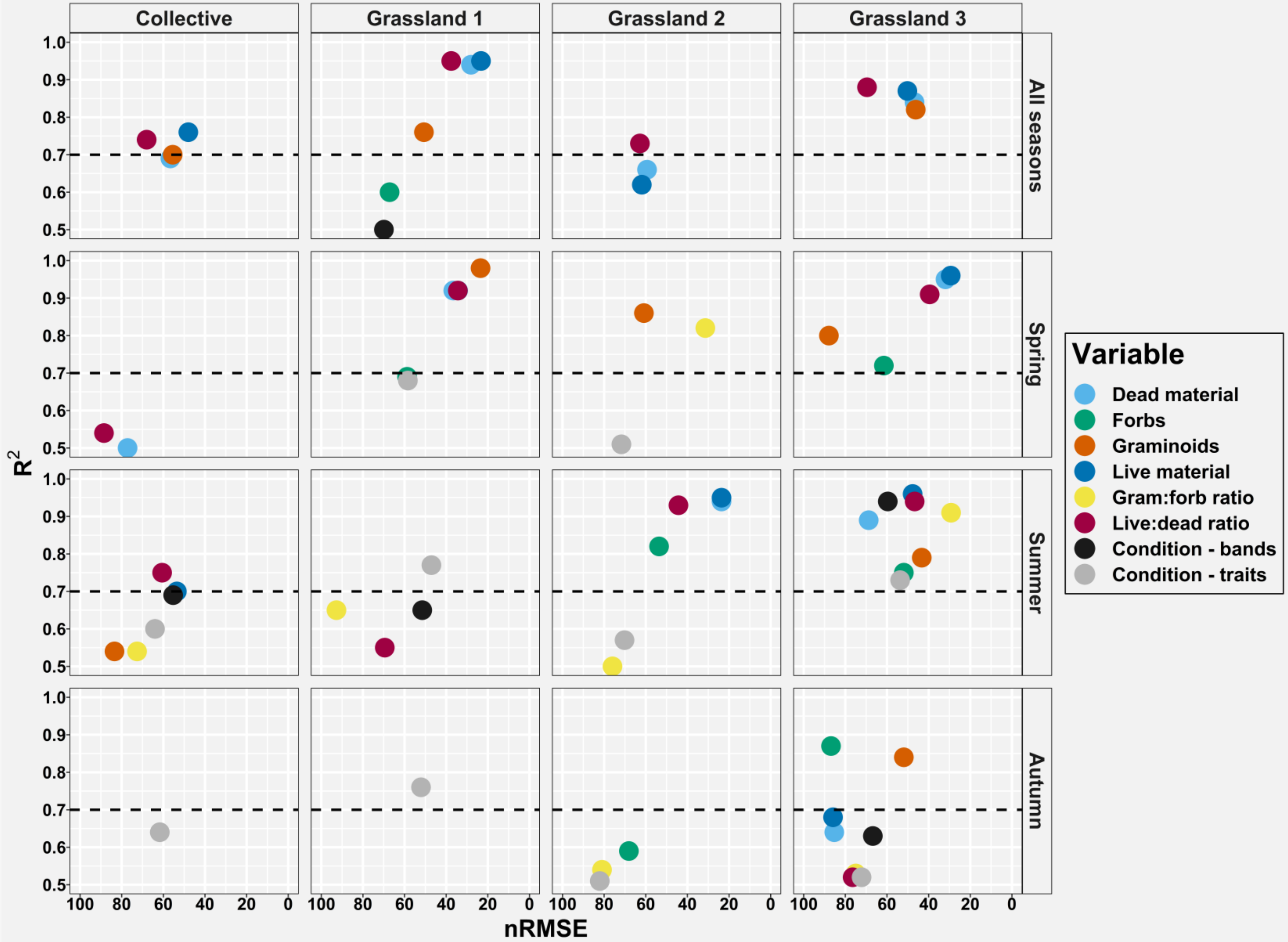


*Figure 5.3: Median results of iterated model runs where spectral data were used to predict CSM-condition and cover-based grassland variables for each of the three seasons (n = 10 or 30) and for all seasons (n = 30 or 90). Also included are the results of predicting CSM-condition with grassland variables data.*

### 5.2.3. Predicting CSM-condition with spectral data or grassland variables

Of 32 model runs where spectral data were used as predictors of CSM-condition (Figures 5.4 and 5.5); 11 produced $R^2$ results => 0.5 and nRMSE <100, 5 of which have $R^2$ results => 0.7. Most of these PLSR models were for Grasslands 1 and 3 (5 and 4 model runs respectively), the other two results being from analysing grasslands collectively. Using FULL spectral data produced 6 PLSR models with $R^2$>0.5 whilst VNIR produced 5 PLSR models with $R^2$>0.5. Using data collected in summer produced far more PLSR models with $R^2$>0.5 (6) than using data from other seasons or analysing data from all seasons collectively (5 model runs in total, 1-2 from each season or from collective analysis).

Of 32 model runs where grassland variables were used to predict CSM-condition (Figures 5.4 and 5.5); 13 of 32 model runs had $R^2$ results >0.5, 4 of which had $R^2$ results => 0.7. Of these 13 model runs, 10 were produced using % cover data but there were no other clear patterns in the results beyond this.

## 5.3. Stability and consistency between model runs using the same response variable

Coefficient of variation (CV) was calculated to evaluate the stability of model performances across sites for specific variables. Figure 5.4 shows the % CV found from the iterated PLSR model runs for the resulting site specific $R^2$ and nRMSE values. Overall, models using cover-based grassland variables produce more consistent $R^2$ results but less consistent nRMSE results than models using mass-based grassland variables. For CSM-condition, this trend is reversed. Whether FULL-based models or VNIR-based models produce more stable results is grassland variable dependent although the results are generally similar.

When using % cover data; model performances for forbs cover, graminoids cover and live:dead ratio cover are relatively stable. When using mass data; model performances for graminoids mass were the most stable with biomass, live material mass, moisture content and live:dead ratio mass also being relatively stable.

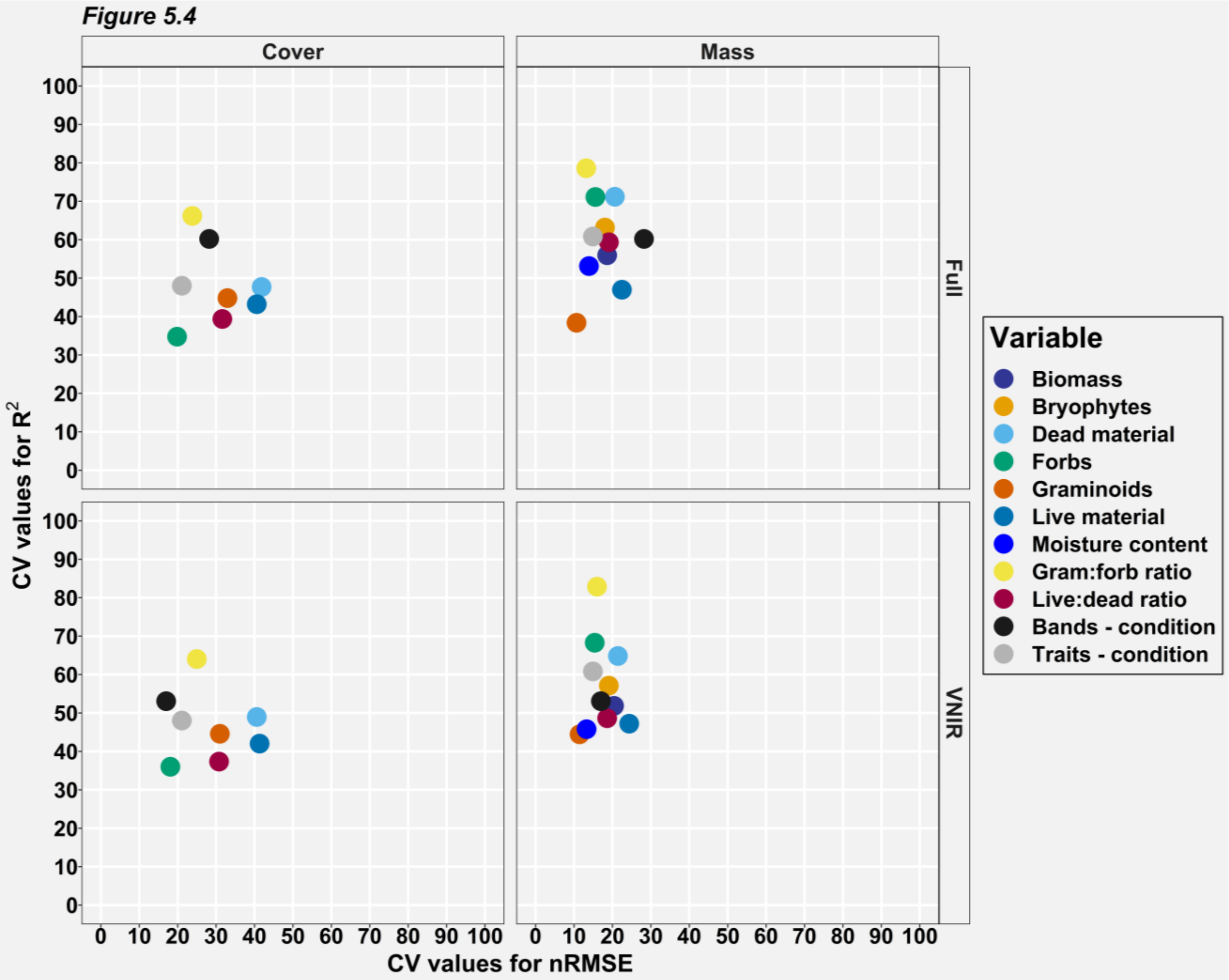



*Figure 5.4: % coefficient of variance (CV) for the $R^2$ and nRMSE results of the site specific PLSR models grouped per treatment and spectral input data.*

## 5.4. VIP analysis for spectral band and grassland variable selection

### 5.4.1. Mass and cover data

Figures 5.5 and 5.6 show the results of using a VIP analysis to understand which spectral bands were the most important predictors for predicting grassland variables, where only important results (=>1) have been included. The results suggest that when using the FULL spectrum, the SWIR bands (1240 and 1640nm) are consistently important whether grasslands are analysed collectively or individually. For Grassland 3, some NIR bands plus 470nm and 647nm were also important. When VNIR spectral data were used; for Grasslands 1-2 plus collective analysis, bands within the 740-860nm were significant. Bands 470nm and 647nm were also important when grasslands were analysed collectively. The results for Grassland 3 were similar to using the FULL spectrum minus the SWIR bands.

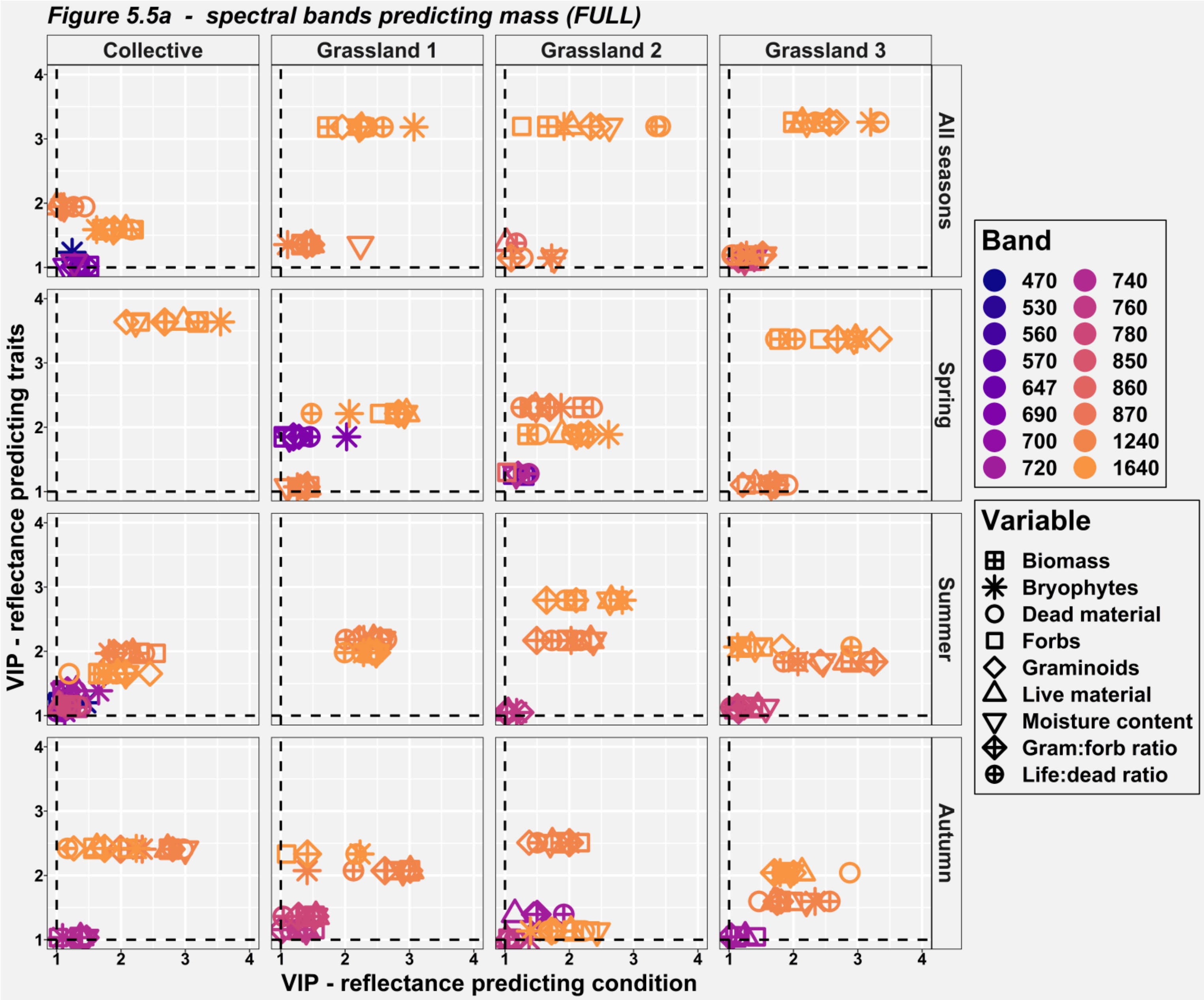


Figure 5.5a - spectral bands predicting mass (FULL)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
VIP - reflectance predicting traits
VIP - reflectance predicting condition
Band
470
530
560
570
647
690
700
720
740
760
780
850
860
870
1240
1640
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Life:dead ratio

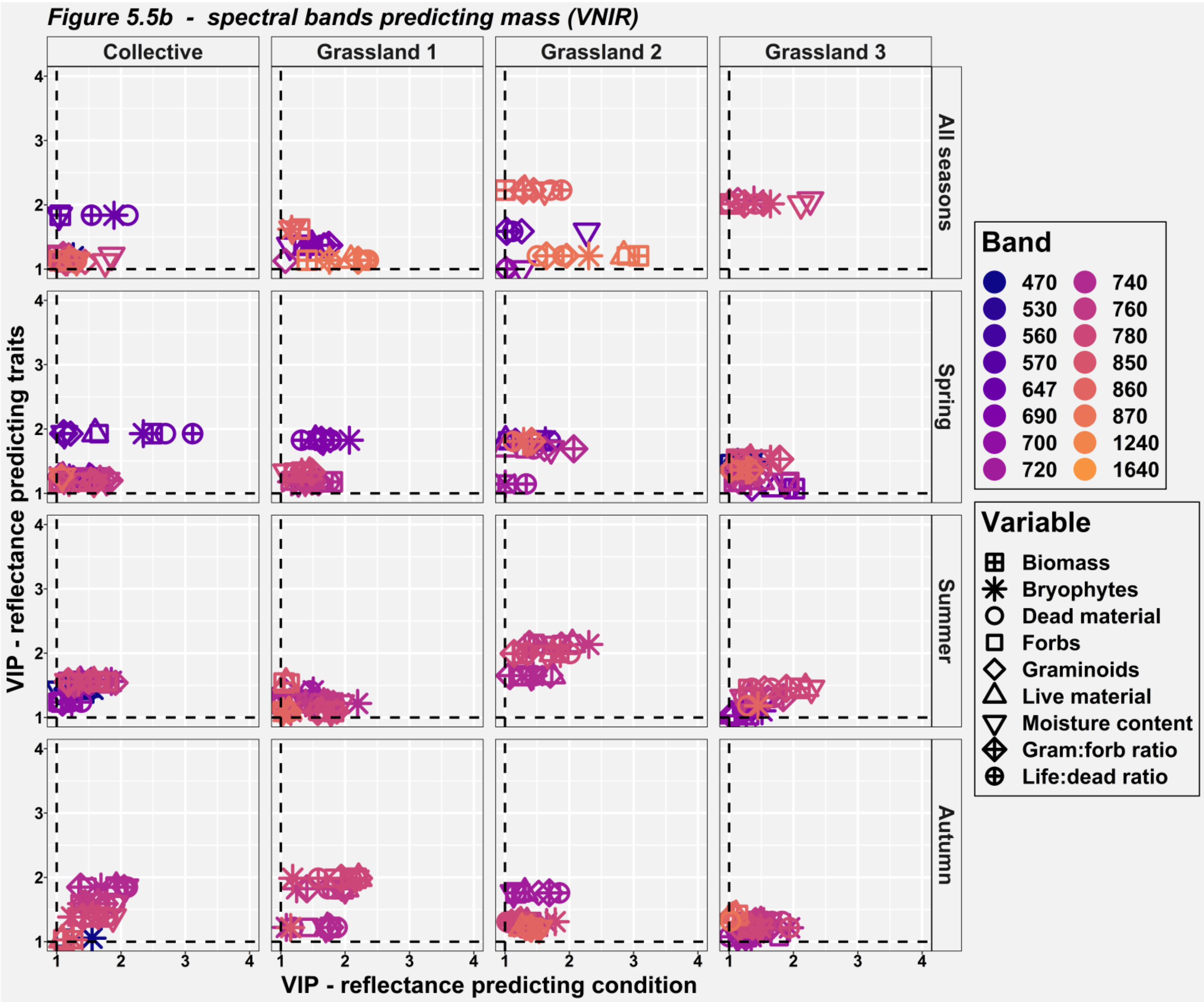


Figure 5.5b - spectral bands predicting mass (VNIR)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
VIP - reflectance predicting traits
VIP - reflectance predicting condition
Band
470
530
560
570
647
690
700
720
740
760
780
850
860
870
1240
1640
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Life:dead ratio

*Figure 5.5: VIP plots showing which combinations of spectral bands (predictors) and which responses (grassland variables on x axis and CSM-condition on y axis) are most important in the study PLSR models where a) PLSR models trained with FULL spectral data and mass-based grassland variables and b) PLSR models trained with VNIR spectral data and mass-based grassland variables.*

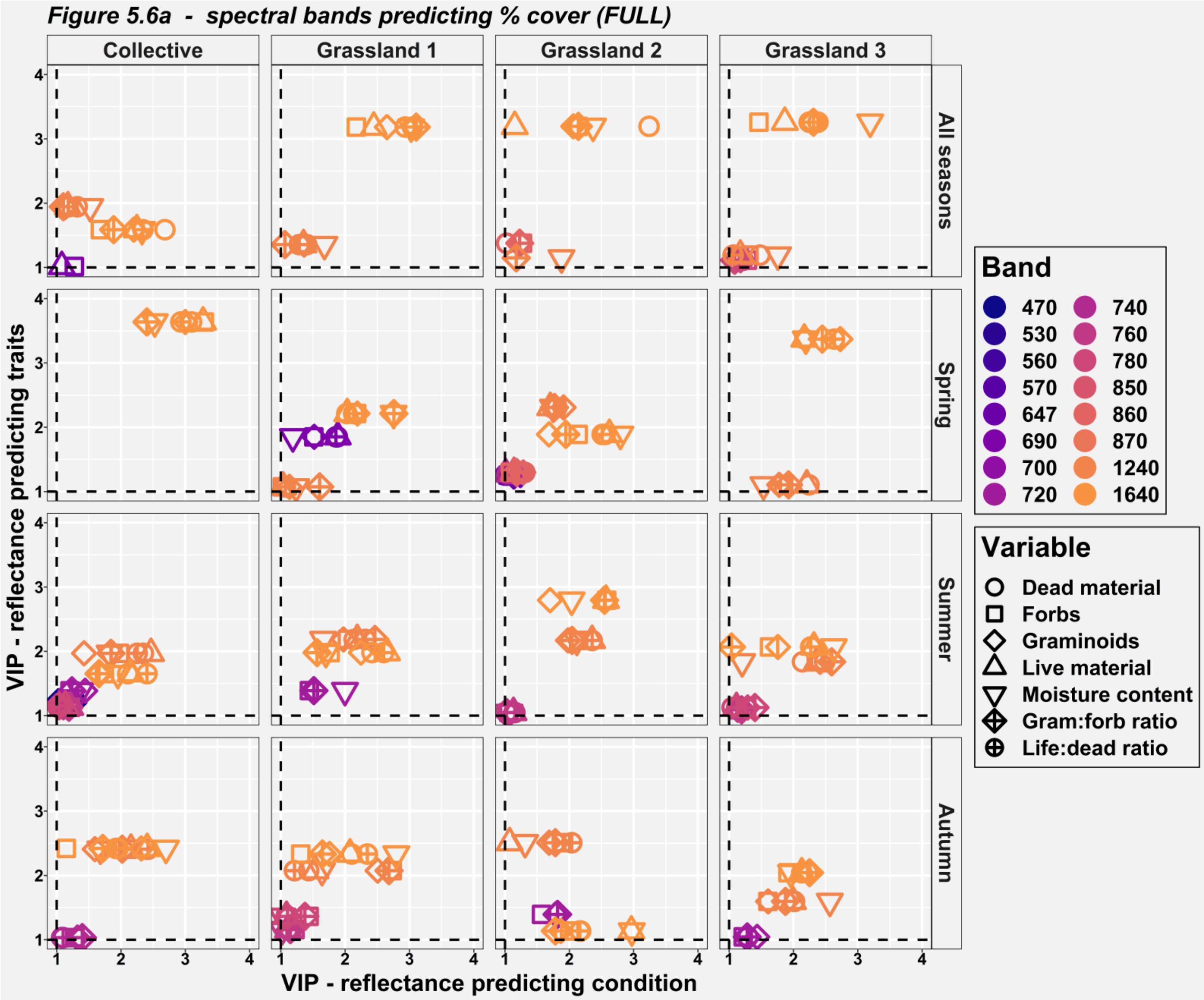


Figure 5.6a - spectral bands predicting % cover (FULL)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
VIP - reflectance predicting traits
VIP - reflectance predicting condition
Band
470
530
560
570
647
690
700
720
740
760
780
850
860
870
1240
1640
Variable
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Life:dead ratio

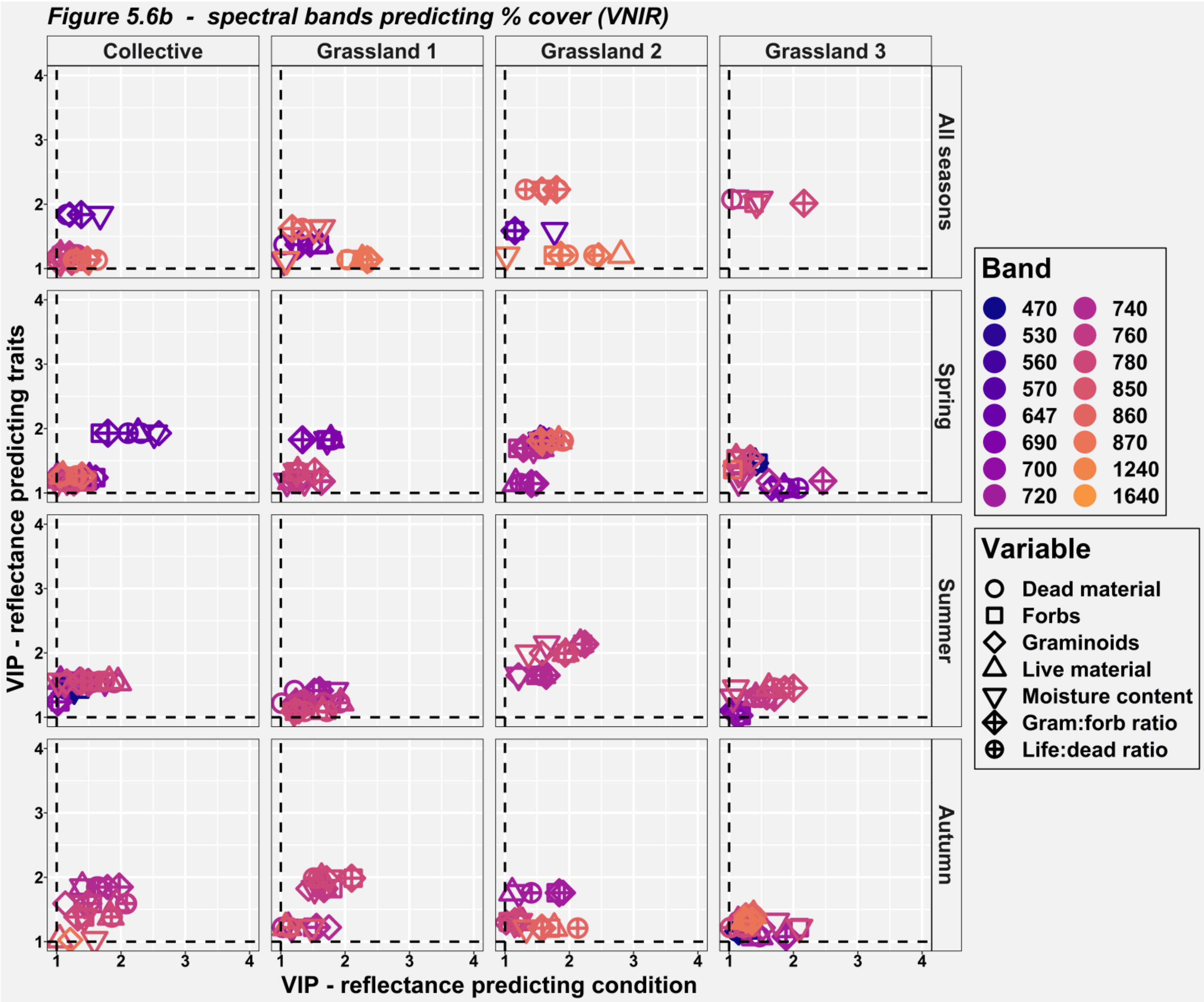
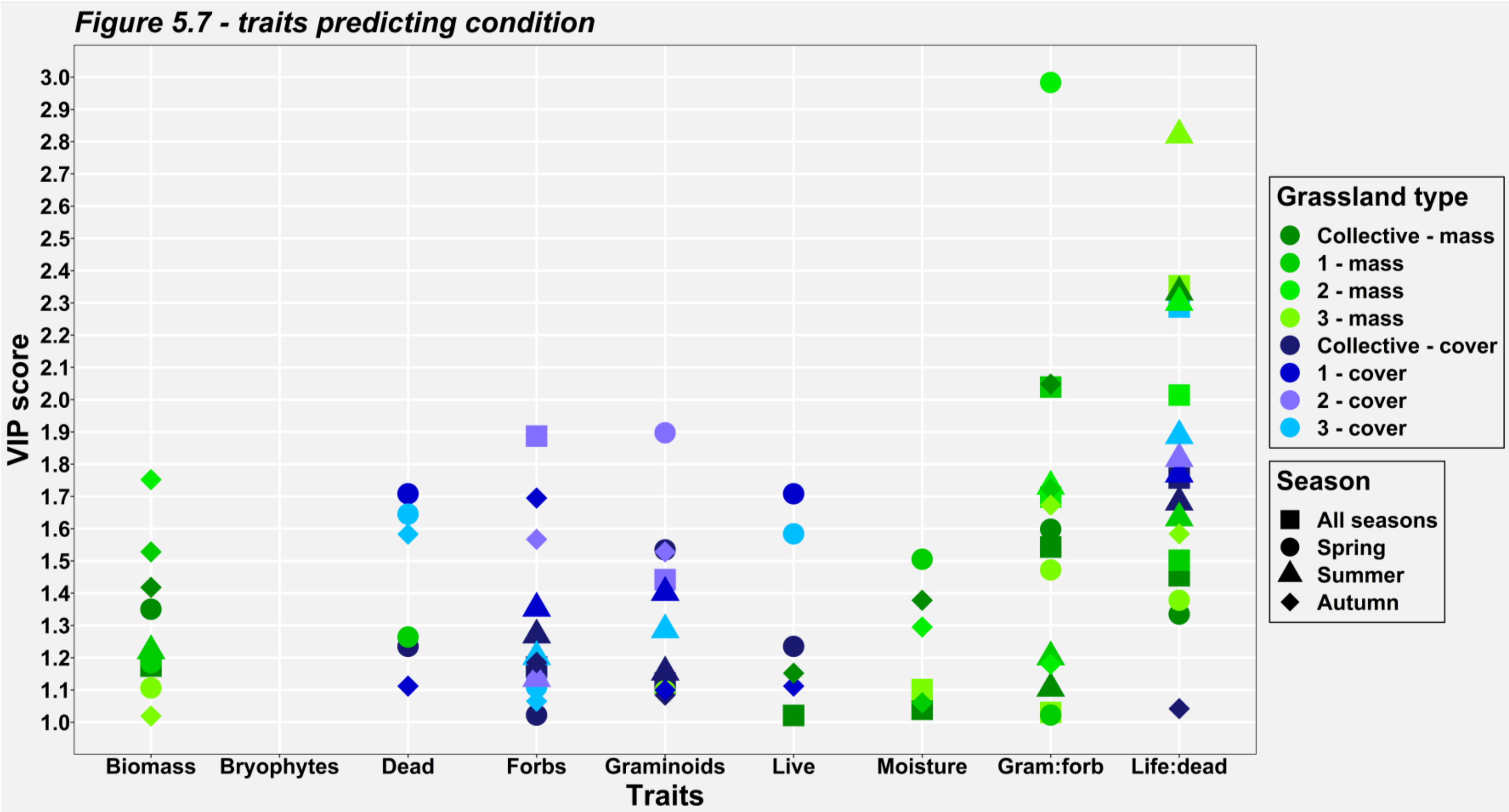


Figure 5.6b - spectral bands predicting % cover (VNIR)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
VIP - reflectance predicting traits
VIP - reflectance predicting condition
Band
470
530
560
570
647
690
700
720
740
760
780
850
860
870
1240
1640
Variable
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Life:dead ratio

*Figure 5.6: VIP plots showing which combinations of spectral bands (predictors) and which responses (grassland variables on x axis and CSM-condition on y axis) are most important in the study PLSR models where a) PLSR models trained with FULL spectral data and cover-based grassland variables and b) PLSR models trained with VNIR spectral data and cover-based grassland variables.*

### 5.4.2. Grassland variables predicting condition

Figure 5.7 shows the results of using grassland variable data to predict CSM-condition. Overall, multiple variables are significant for predicting condition but these grassland variables are different depending on whether mass or cover data are used. When mass data were used, the most important grassland variables were biomass, gram:forb ratio mass, live:dead ratio mass and moisture content. Primarily; forbs cover and graminoids cover were important when cover data were used although dead material cover, live material cover and live:dead ratio cover also had importance. These trends exist when analysing data from any one season or for all seasons.

2767 


2768 *Figure 5.7: VIP plot showing which grassland variables are most important in predicting CSM-condition using either mass- or cover-*
2769 *based grassland variables from analysing grasslands individually or collectively or for one or all seasons.*

## 5.5. Comparison of PLSR models trained with actual data and PLSR models trained with random data

The median values of $R^2$ and nRMSE results presented in Figures 5.2 and 5.3 (i.e. actual models) were compared against the results of 999 further model runs with randomised response variable values (randomised models) to test if the results run with the actual data genuinely produce reliable results. The results of comparing actual models to randomised models can be seen in Figures 5.8 and 5.9, where actual models that beat at least 950 randomised models (95% level) are considered consistently superior to randomised models.

These results suggest that producing actual models that are superior to randomised models depends on the quantity of data being used but also whether data were collected over one season or multiple seasons. When data from all three grasslands and for all seasons (n = 90) are used, the median $R^2$ and nRMSE results are consistently superior to randomised models. When grassland data are analysed collectively for all grasslands and one season, almost all median nRMSE results, and median $R^2$ results for a few grassland variables, produces results that are consistently superior to results from randomised models at 95% level though some grassland variables are at least consistently superior to results from randomised models at an 80% level. When data from one grassland and one season are used (n = 10) or all seasons and one grassland (n = 30), the actual models are no more robust than randomised models.

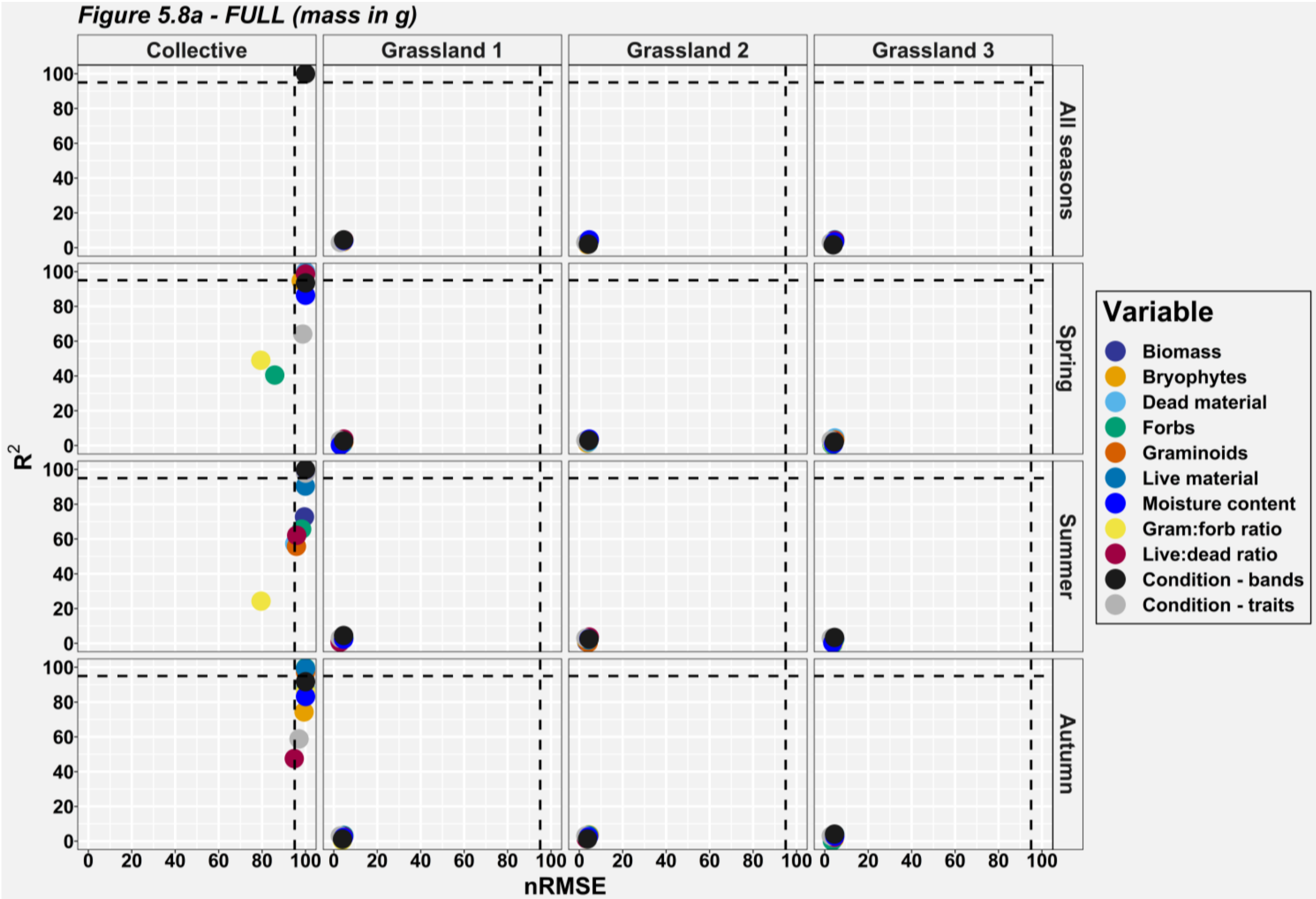


Figure 5.8a - FULL (mass in g)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
0
20
40
60
80
100
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

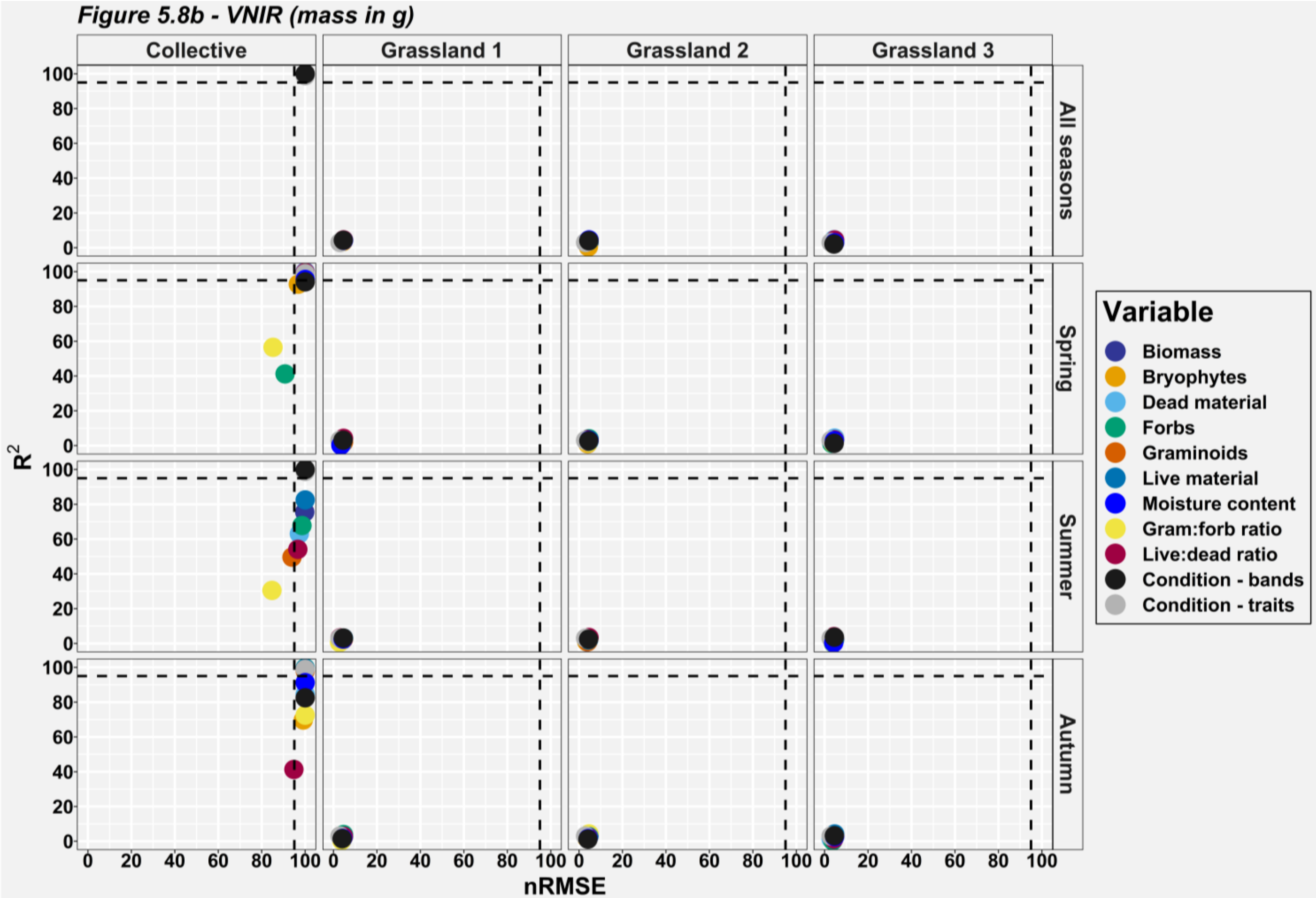



*Figure 5.8: Rankings of the median values of iterated model runs using actual mass response data and also iterated model runs using randomised response data, where rankings >95% level are considered significant for the actual model fit.*

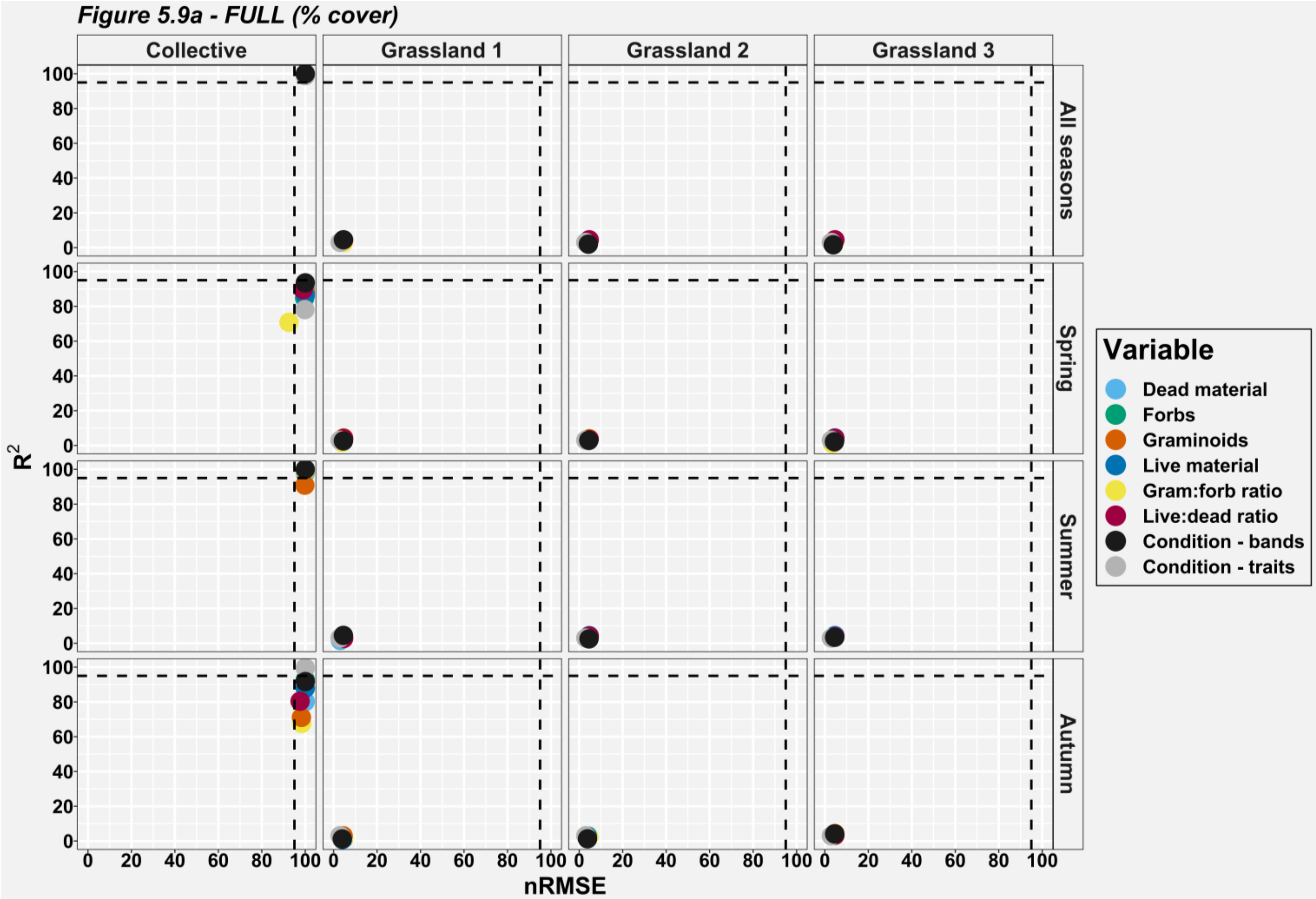
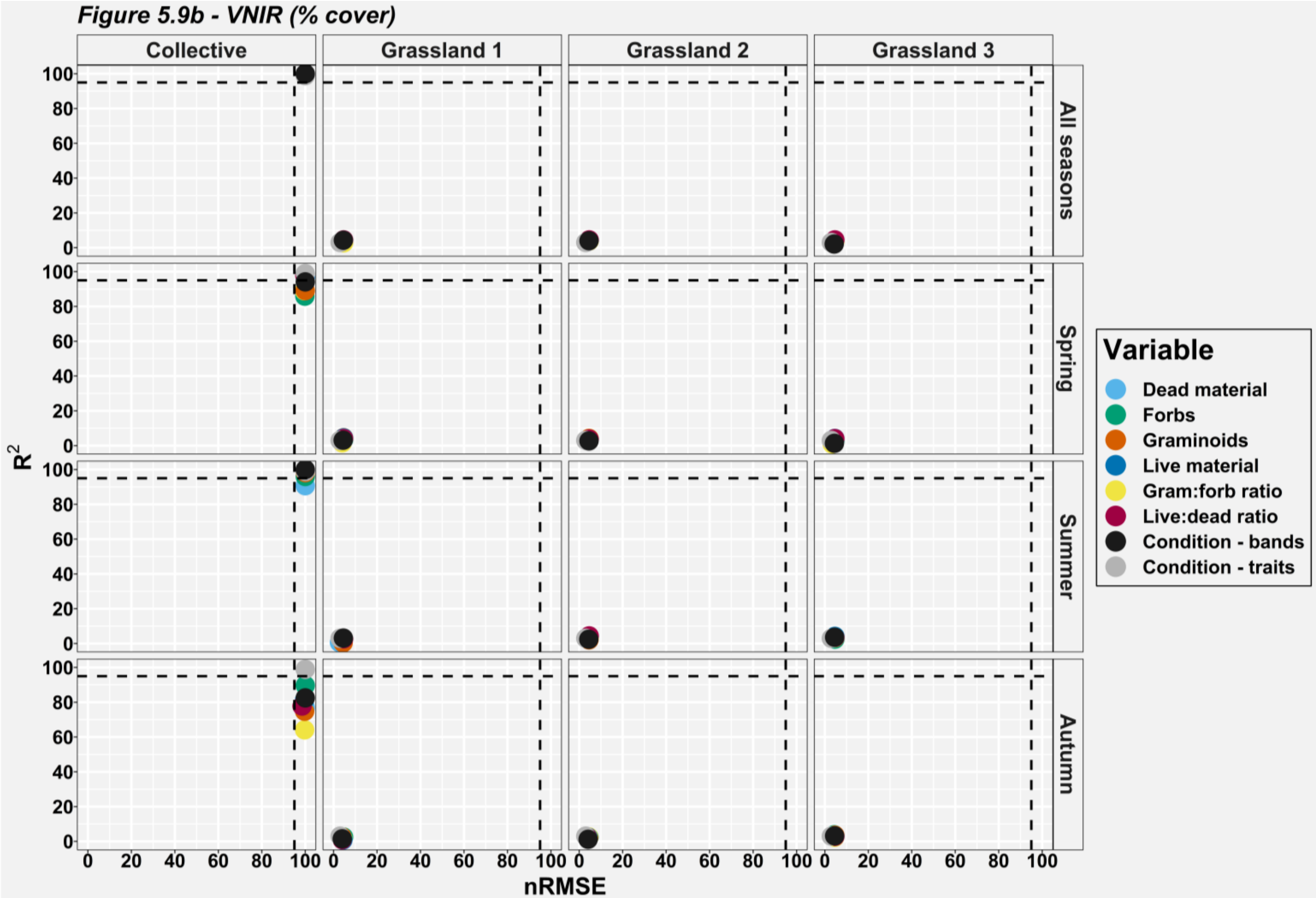


Figure 5.9a - FULL (% cover)
Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R²
nRMSE
0 20 40 60 80 100
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

2797

2798 


2799 *Figure 5.9: Rankings of the median values of iterated model runs using actual % cover response data and iterated model runs using*
2800 *randomised response data, where rankings >95% are considered consistently superior to randomised models*

# Chapter 6 - Comparison of patch level (1m$^2$) spectral data from different devices and an assessment using field level (200x1m) CROPSCAN data when predicting condition-related grassland variables on calcareous semi-natural grasslands

## 6.1. Grassland site characteristics

The boxplots of Figure 6.1 show the quantity of each grassland variable for each grassland together with the results of significant difference tests between grassland types, using an unpaired two-sample Wilcoxon test. This differs from a similar projection in Chapter 5 (Figure 5.1) in that only data collected during the summer are analysed. Overall, the Wilcoxon tests for grassland variables show that some grassland variables are significantly different at least between two grasslands. The Wilcoxon tests for the mass-based grassland variables show that for biomass, forbs mass and live material mass; two grasslands are significantly different from one other grassland. For dead material mass and moisture content; two grasslands are significantly different from one other grassland and one grassland from two others. For bryophytes mass, all grasslands are significantly different from each other. The Wilcoxon tests for the cover-based grassland variables show that for dead material cover, live material cover and live:dead ratio cover; two grasslands are significantly different from one other grassland and one grassland from two others.

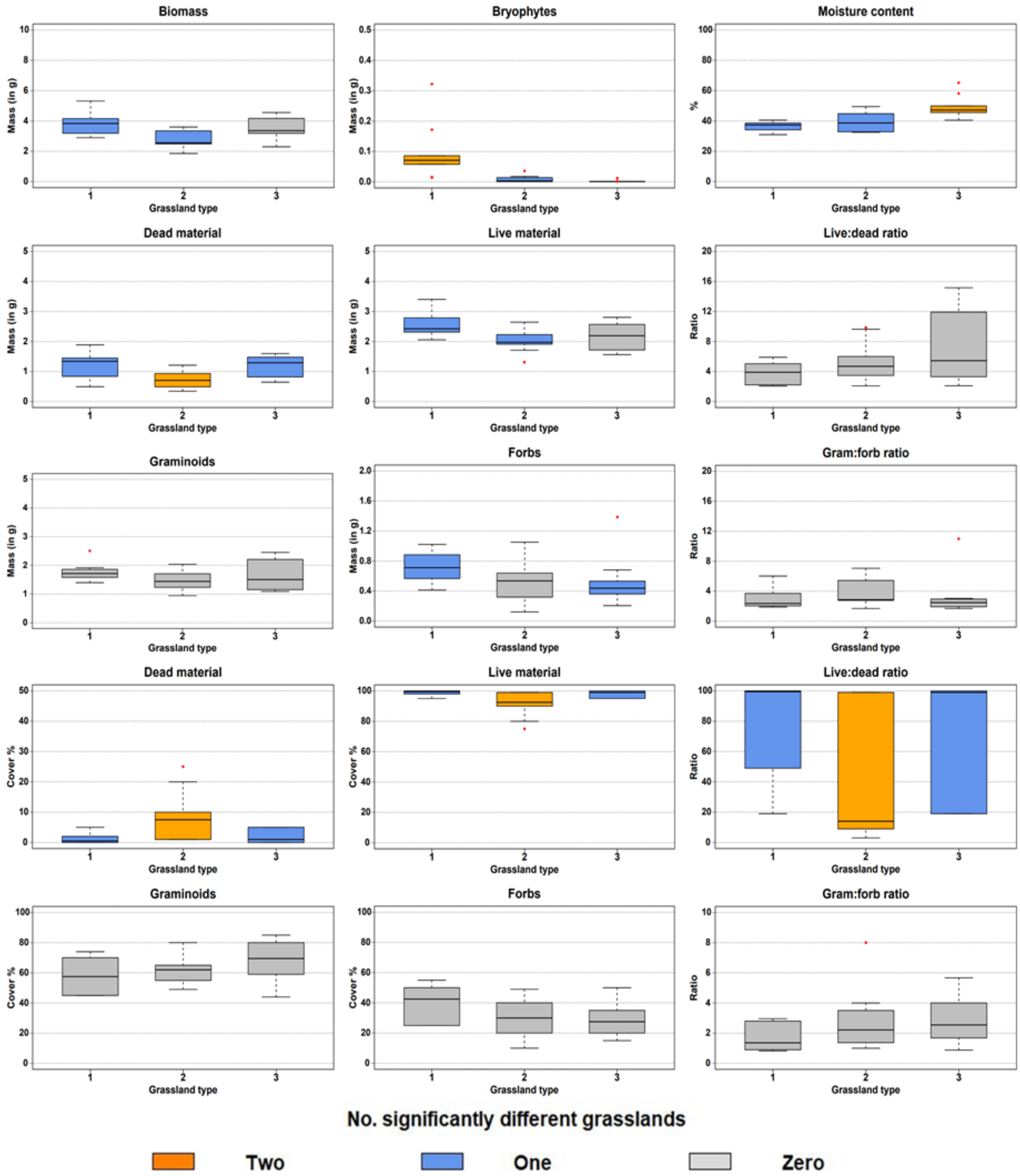



*Figure 6.1: Boxplots of the grassland variable values for the three grassland sites. The boxplot colours summarise the unpaired two-sample Wilcoxon test results between grassland types where the colour represents the number of sites from which each grassland variable is significantly different (p<0.05).*

## 6.2. Predicting grassland variables and condition using PLSR

The median $R^2$ and nRMSE results of the PLSR modelling from the iterated model runs to predict mass, % cover grassland variables and CSM-condition using spectral data from the three different devices as predictors where $R^2$ => 0.5 and nRMSE <= 100 can be seen in Figures 6.6 and 6.7, with the full results presented in Appendix Figure 5. Overall; when PLSR models were trained with data from all three grasslands (n = 30), using spectral data from different devices produced similar results. When PLSR models were trained with data from a single site (*n* = 10); there is no set pattern in the results as performance seems to be specific to the grassland and the spectral device used.

### 6.2.1. Predicting mass-based grassland variable data

When grasslands are analysed collectively using spectral data from any device (Figure 6.2); bryophytes mass, moisture content and CSM-condition all produced $R^2$ results >0.5 (most are >0.7) and nRMSE <100 when using data from the Rikola camera. When grasslands are analysed individually; most of the significant results came from using spectral data from the Rikola camera, CROPSCAN and the SVC when using data from Grassland 1 plus from Grassland 3 when using a CROPSCAN.

### 6.2.2. Predicting cover-based grassland variable data

When grassland were analysed collectively using spectral data from any device (Figure 6.3); most grassland variables produced $R^2$ values => 0.5 and nRMSE <100 for at least one device but CSM-condition, live material cover, live:dead ratio cover produced significant results for all three devices with live material cover and CSM-condition producing $R^2$ results >0.7. When grasslands were analysed individually using spectral data from any device; most grassland variables produced significant results except for Grassland 1 when using spectral data from the SVC.

### 6.2.3. Predicting CSM-condition using grassland variables

Of 12 model runs when using spectral data to predict CSM-condition (Figures 6.6 and 6.7); 8 produced $R^2$ results => 0.5 and nRMSE <100, 4 of which have $R^2$ results => 0.7. Most of the significant results were produced when analysing grasslands collectively (3) whilst analysing grasslands individually produced 1-2 significant results. Using different devices produced 2 results for the SVC and 3 significant results each for the CROPSCAN and Rikola camera. Of 8 model runs when using grassland variables to predict CSM-condition; 4 produced $R^2$ results => 0.5 and nRMSE <100, 2 of which have $R^2$ results => 0.7. All significant results using % cover data. Analysing grasslands collectively or individually produced 1 significant result each.

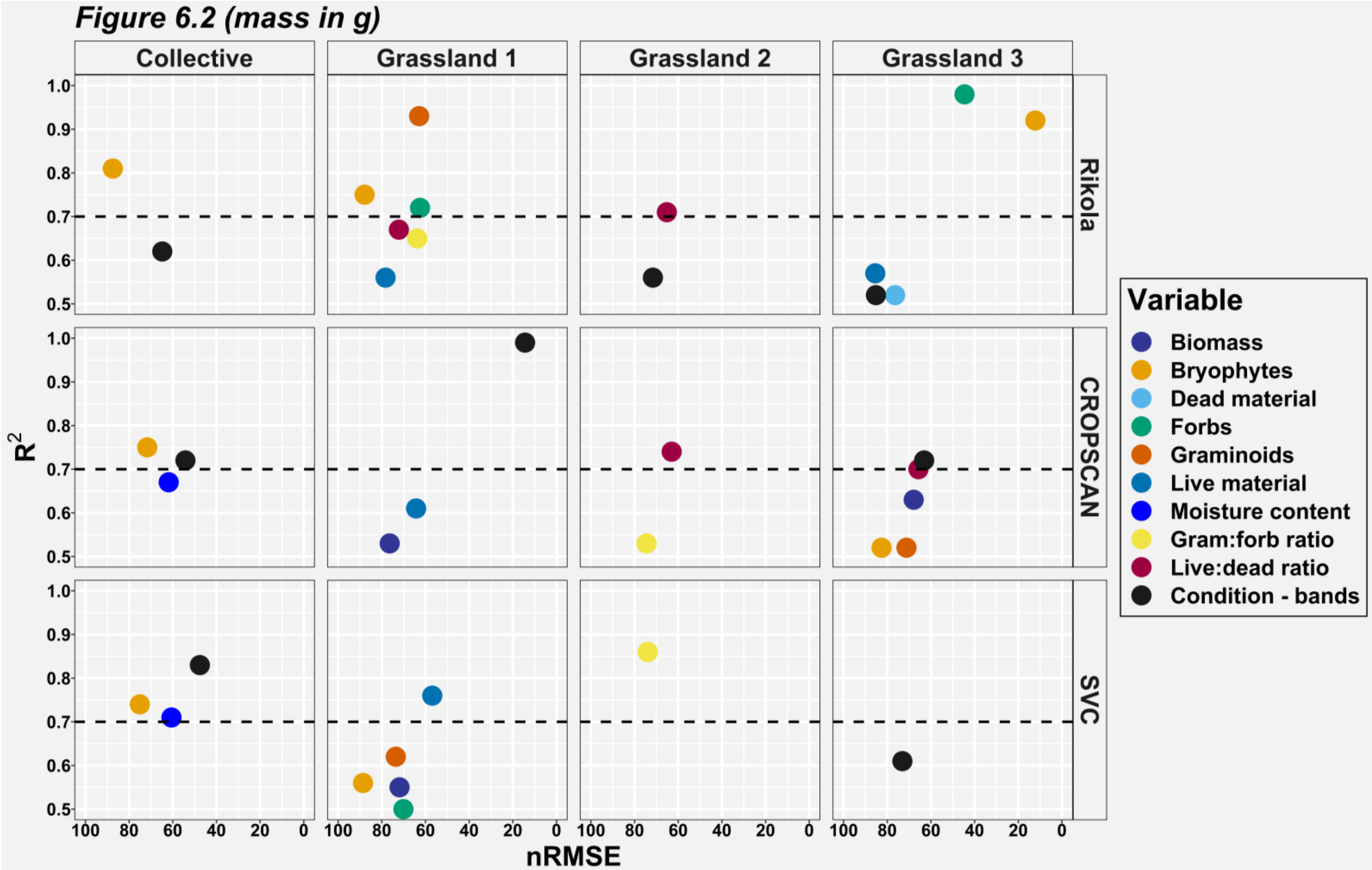
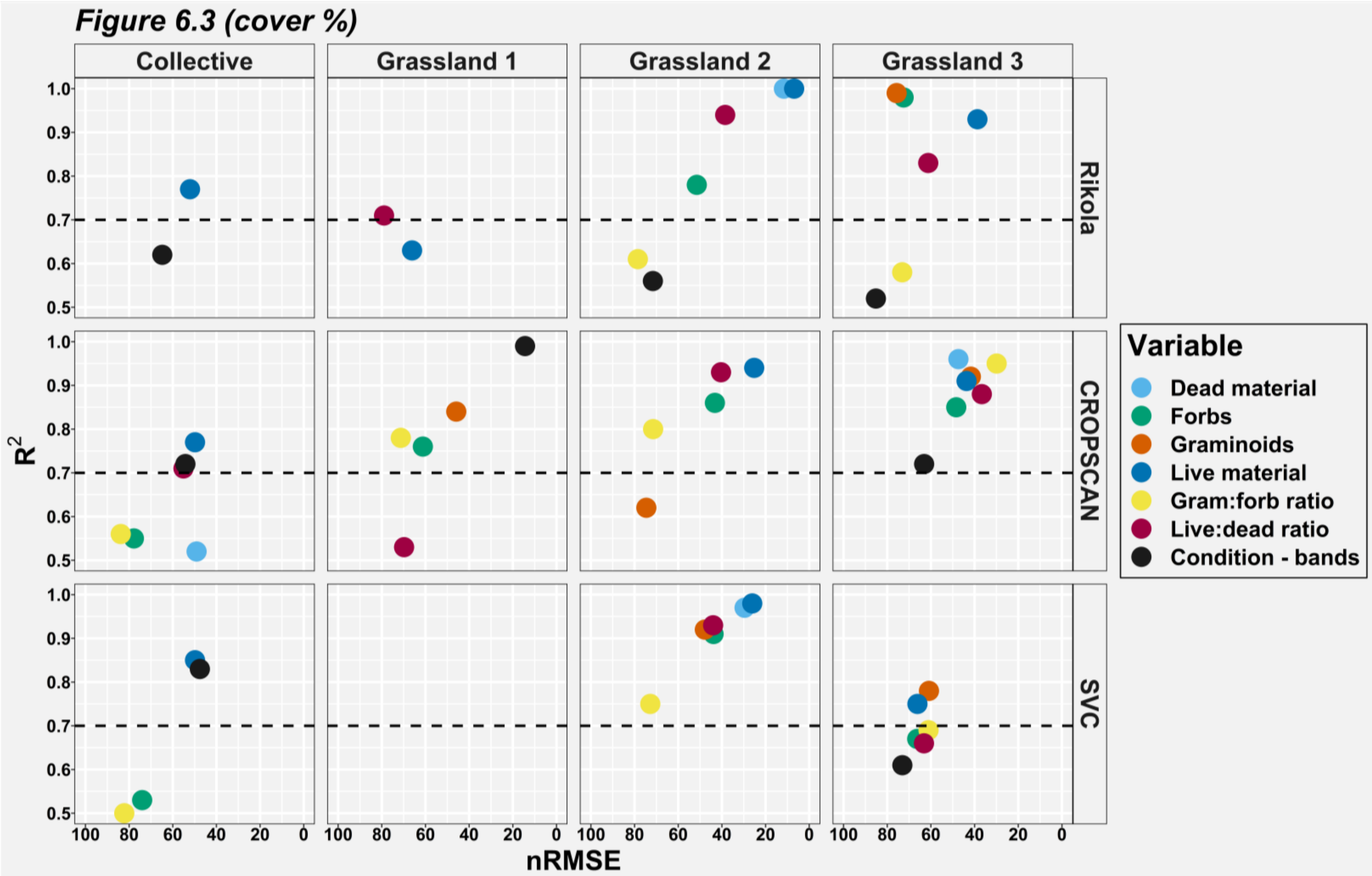



Figure 6.2: *Median results of iterated model runs where spectral data from three different devices were used to predict CSM-condition and mass-based grassland variables for all grasslands collectively (n = 30) or single sites (n = 10).*




2875

2876 Figure 6.3: *Median results of iterated model runs where spectral data from three different devices were used to predict CSM-condition and*
2877 *cover-based grassland variables for all grasslands collectively (n = 30) or single sites (n = 10).*

## 6.3. Comparing observed and predicted values

Each of the trained PLSR models produced predicted values for each grassland variable on each quadrat. These predicted values have been plotted against the observed values (1:1 lines have been included) for comparison in the appendix. The clusters of some grassland variables appear to be close to the 1:1 line. For other grassland variables, the 1:1 line appears to run closer to the main body of the cluster than to the lowest and/or highest observed values, suggesting that the PLSR models did not predict these values as accurately. For a few grassland variables, particularly live:dead ratio cover, the clusters appear to be scattered suggesting a low predictive power of the associated PLSR models.

## 6.4. Extrapolating predicted grassland variables and condition using CROPSCAN data as predictors

Moderate to strong fitting PLSR models trained with data from all three grasslands collectively using CROPSCAN data as predictors were used to predict grassland variable values at field level (Figure 6.4).

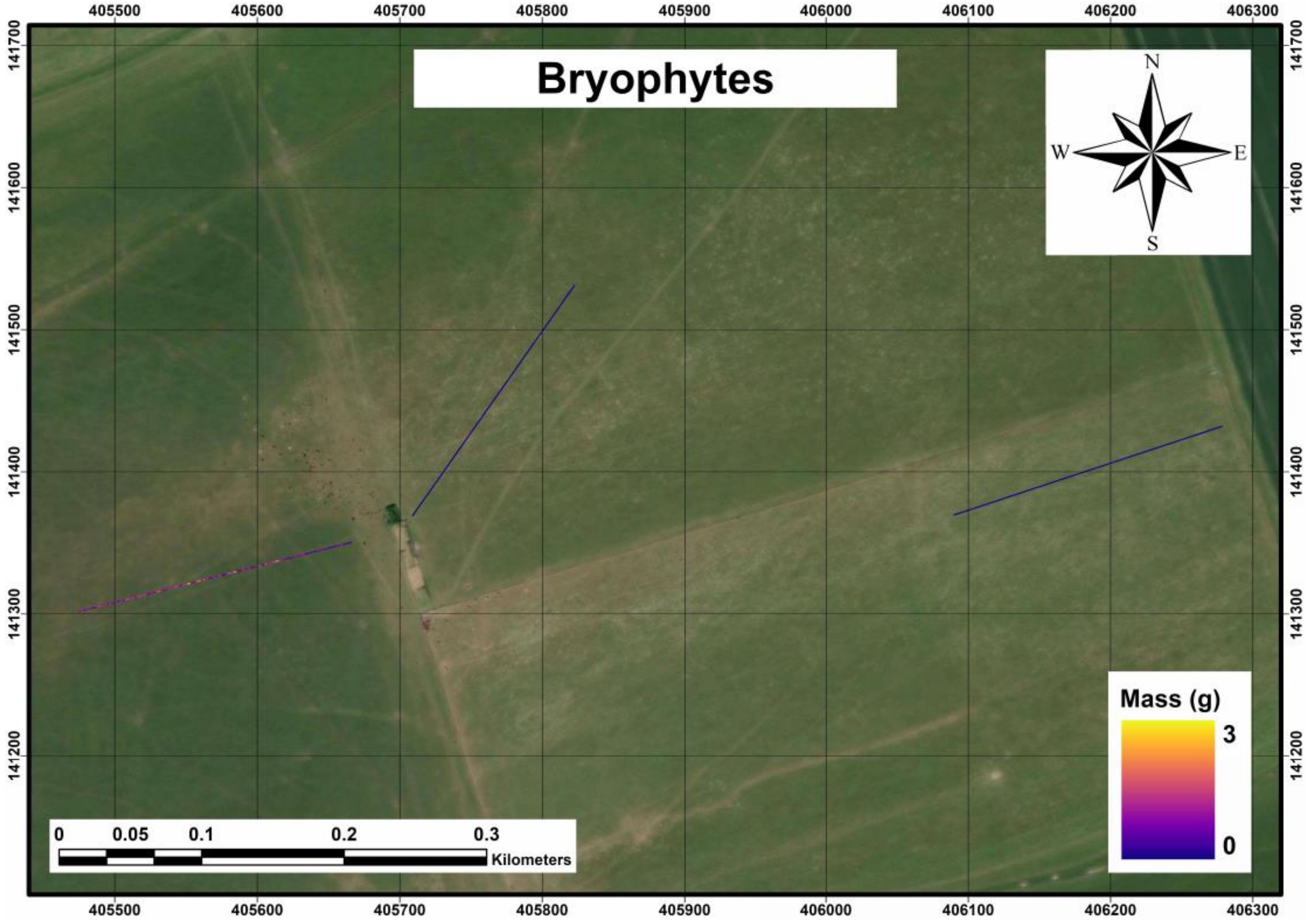



Figure 6.4a: Projection of bryophyte mass predicted values derived from a PLSR model trained with CROPSCAN spectral data.

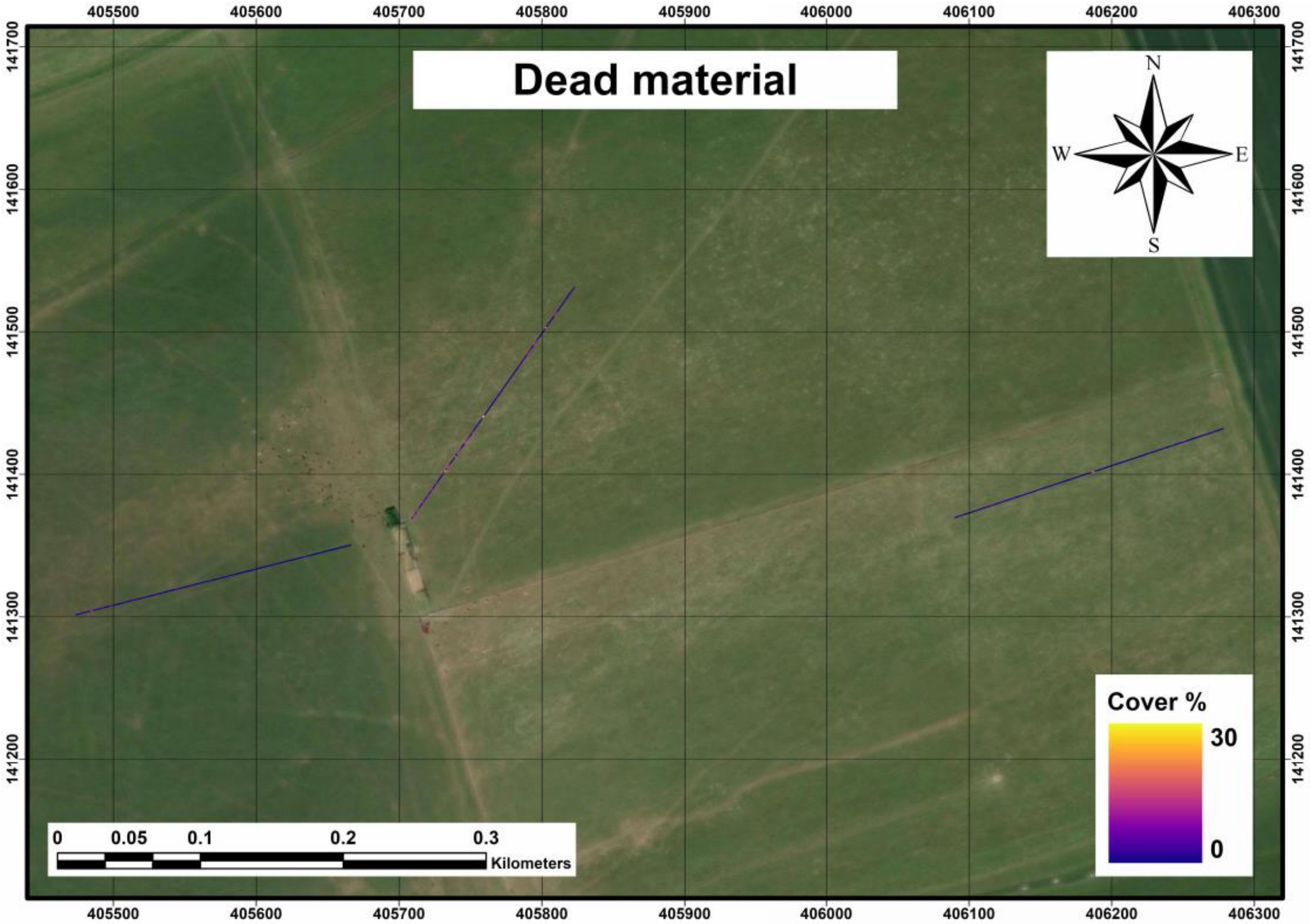
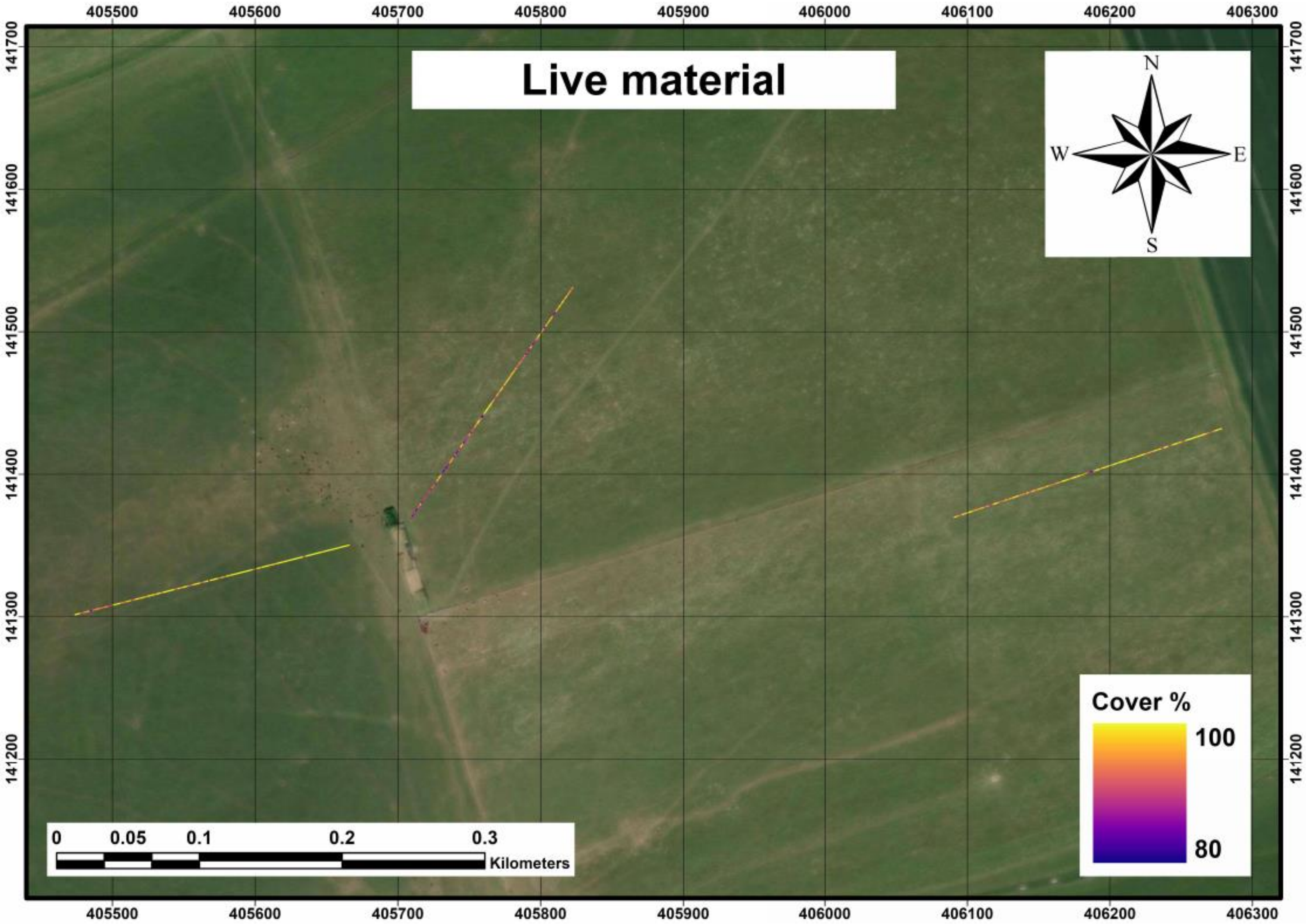



Figure 6.4b: Projection of dead material % cover predicted values derived from a PLSR model trained with CROPSCAN spectral data.

2898 


2899 Figure 6.4c: Projection of live material % cover predicted values derived from a PLSR model trained with CROPSCAN spectral data.

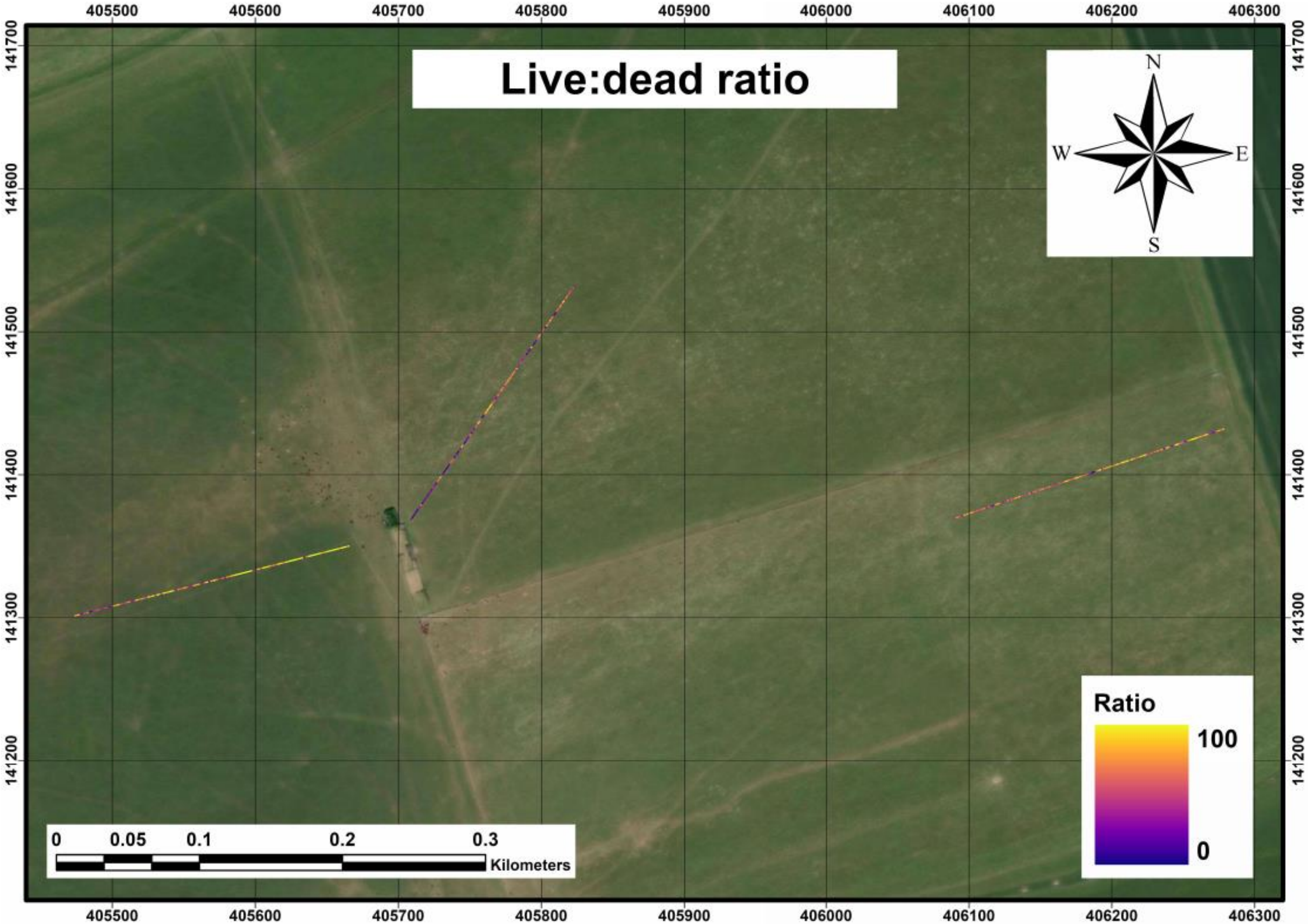
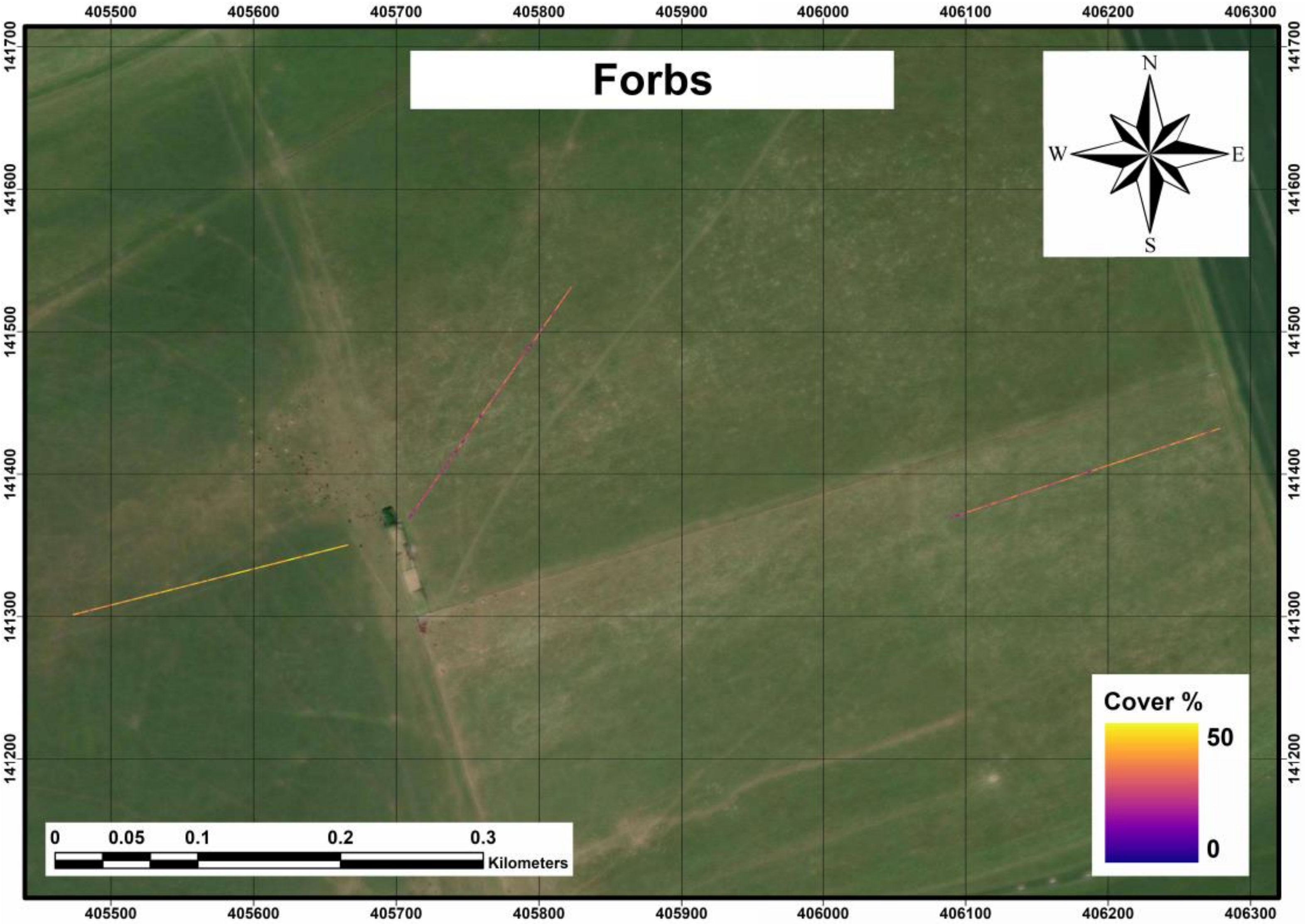
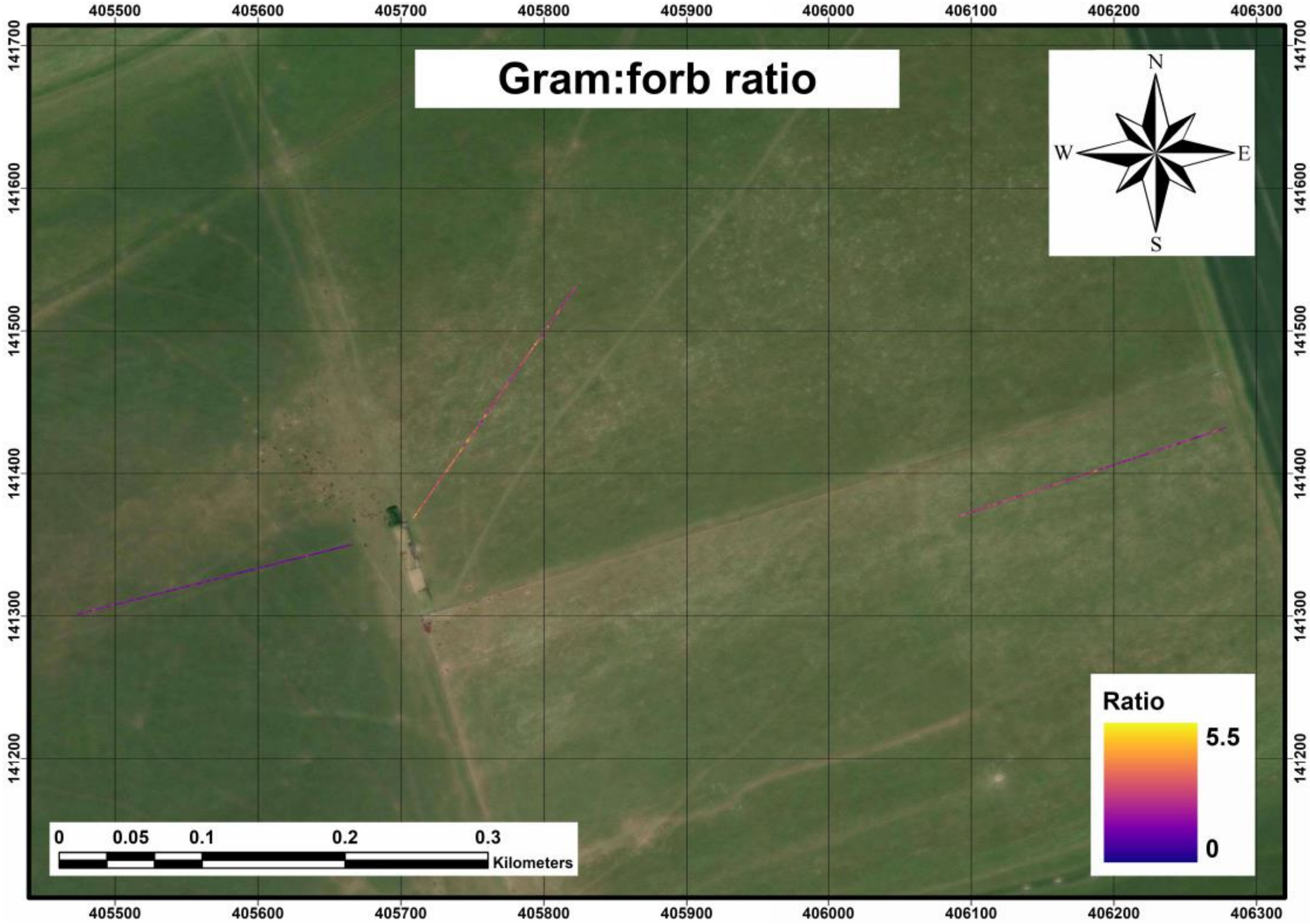


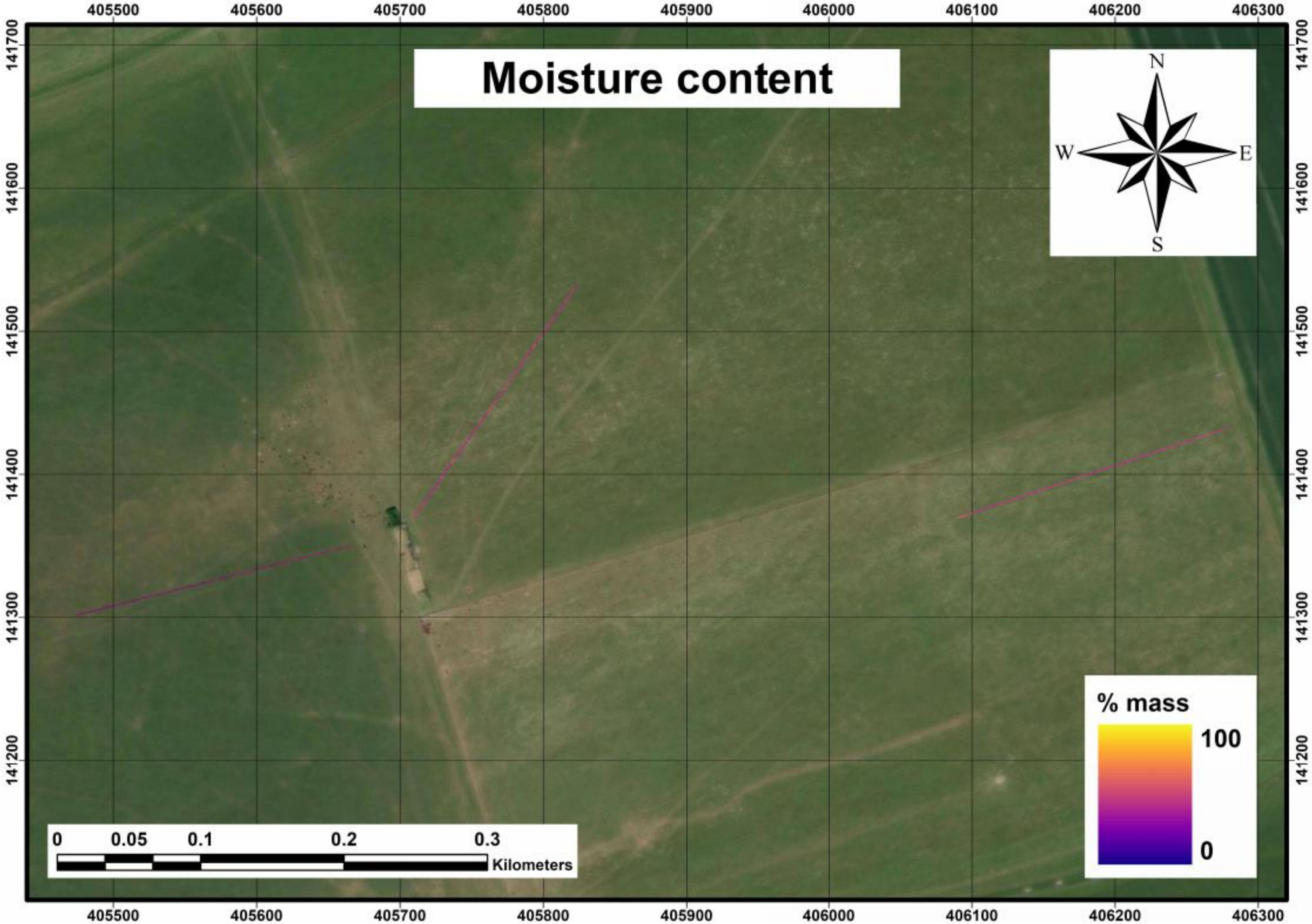

Figure 6.4d: Projection of live:dead ratio % cover predicted values derived from a PLSR model trained with CROPSCAN spectral data.

2902 

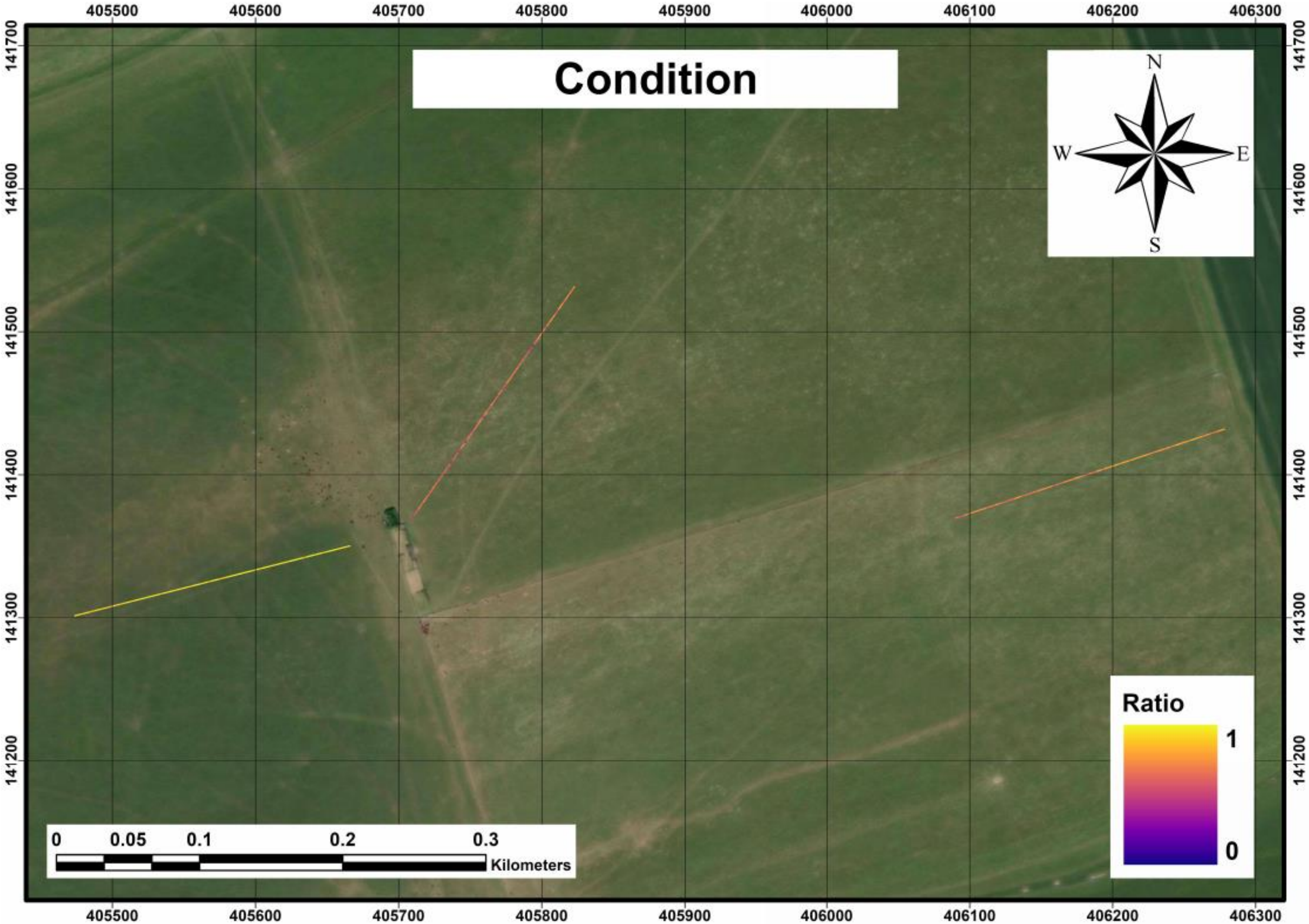

2903 Figure 6.4e: Projection of forbs % cover predicted values derived from a PLSR model trained with CROPSCAN spectral data.

2904 


2905 Figure 6.4f: Projection of gram:forb ratio % cover predicted values derived from a PLSR model trained with CROPSCAN spectral data.

2906 


2907 Figure 6.4g: Projection of moisture content (% mass) predicted values derived from a PLSR model trained with CROPSCAN spectral data.

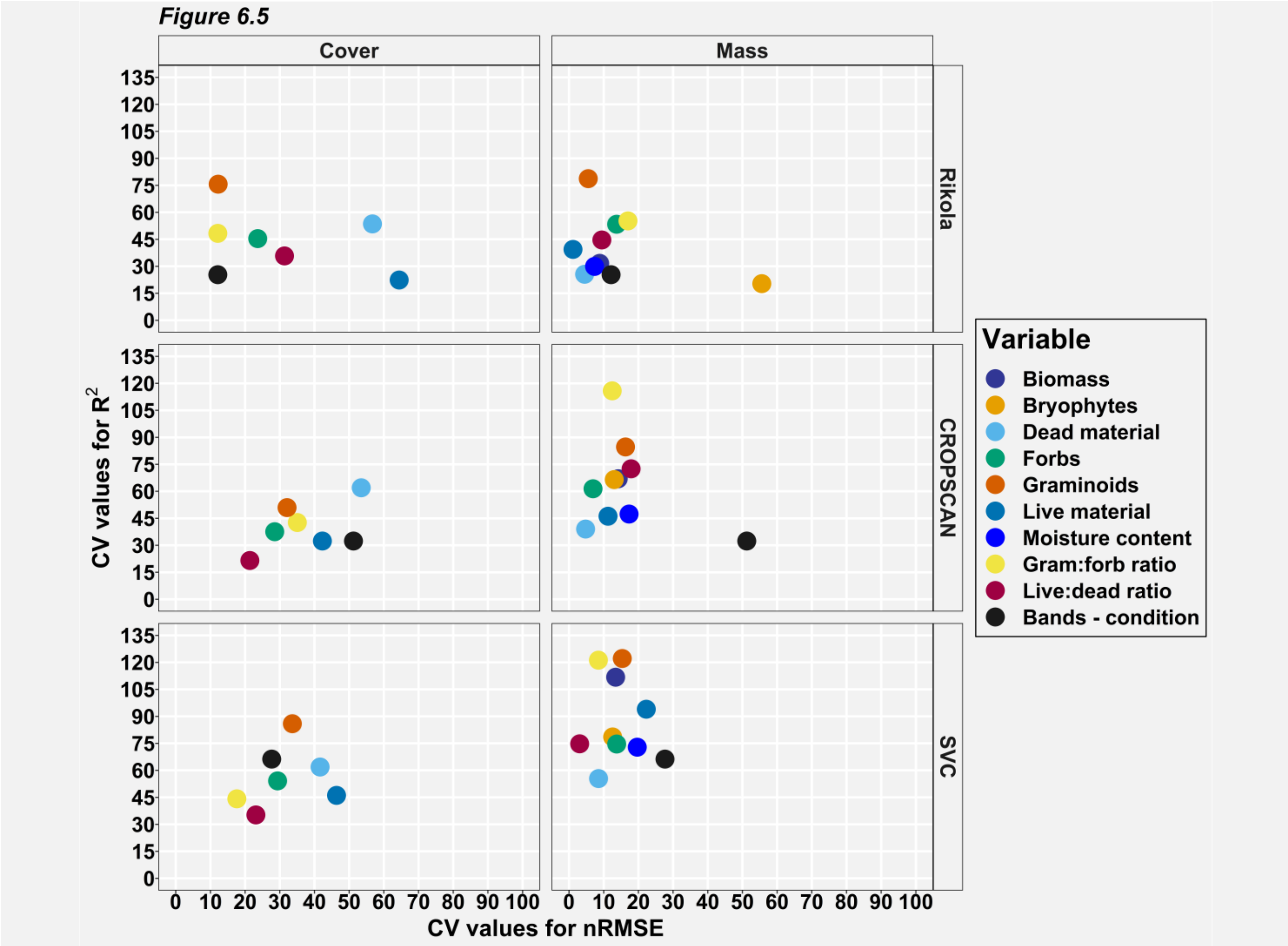
2908 


2909 Figure 6.4h: Projection of CSM-condition predicted values derived from a PLSR model trained with CROPSCAN spectral data.

## 6.5. Stability and consistency between model runs using the same response variable

Figure 6.5 shows the % CV of the median found from the iterated PLSR model runs and the resulting $R^2$ and nRMSE values of the site specific PLSR models that were calculated to evaluate the stability of model performances across sites for specific grassland variables. Lower CV values were considered to be more indicative of model stability. Overall, models predicting mass-based grassland variables produce more consistent $R^2$ results but less consistent nRMSE results than models predicting % cover-based grassland variables.

The results between different spectral devices appear to be similar when predicting mass-based grassland variables and for most grassland variables when predicting cover-based grassland variables, with some of the grassland variables showing a different level of consistency when spectral data from the Rikola VNIR camera are used as predictors. When predicting % cover data, forbs cover, gram:forb ratio cover and live:dead ratio cover appear to be relatively consistent. When predicting mass data, dead material mass and moisture content are relatively consistent for all three devices. Other grassland variables are relatively consistent for the two devices; forbs mass, live material mass and live:dead ratio mass.




2928

2929 Figure 6.5: *% coefficient of variation (CV) for the $R^2$ and nRMSE results of the site specific PLSR models grouped per treatment and spectral*
2930 *input data from different spectral devices.*

## 6.6. VIP analysis for spectral band selection

Figures 6.6 and 6.7 show the results of VIP analysis, highlighting the spectral regions most important for predicting grassland variables (by mass or by % cover) and CSM-condition. For this analysis, the spectral bands were grouped into the following categories: VIS (300-700nm), NIR (701-900nm), SWIR1 (901-1640nm) and SWIR2 (1640-2500nm). VIP values >1 were considered to be indicative of a strong predictor variable. The most significant region of the spectral signature for predicting any grassland variable depended on the spectral range of the device. In broad terms, for each device the outer part of the spectrum was most important. When using spectral data from the Rikola camera; the NIR part of the spectrum was most significant except for Grassland 2 where the VIS part of the spectrum was more significant for most grassland variables. When using spectral data from the CROPSCAN or SVC, the NIR and SWIR parts of the spectrum were generally more important.

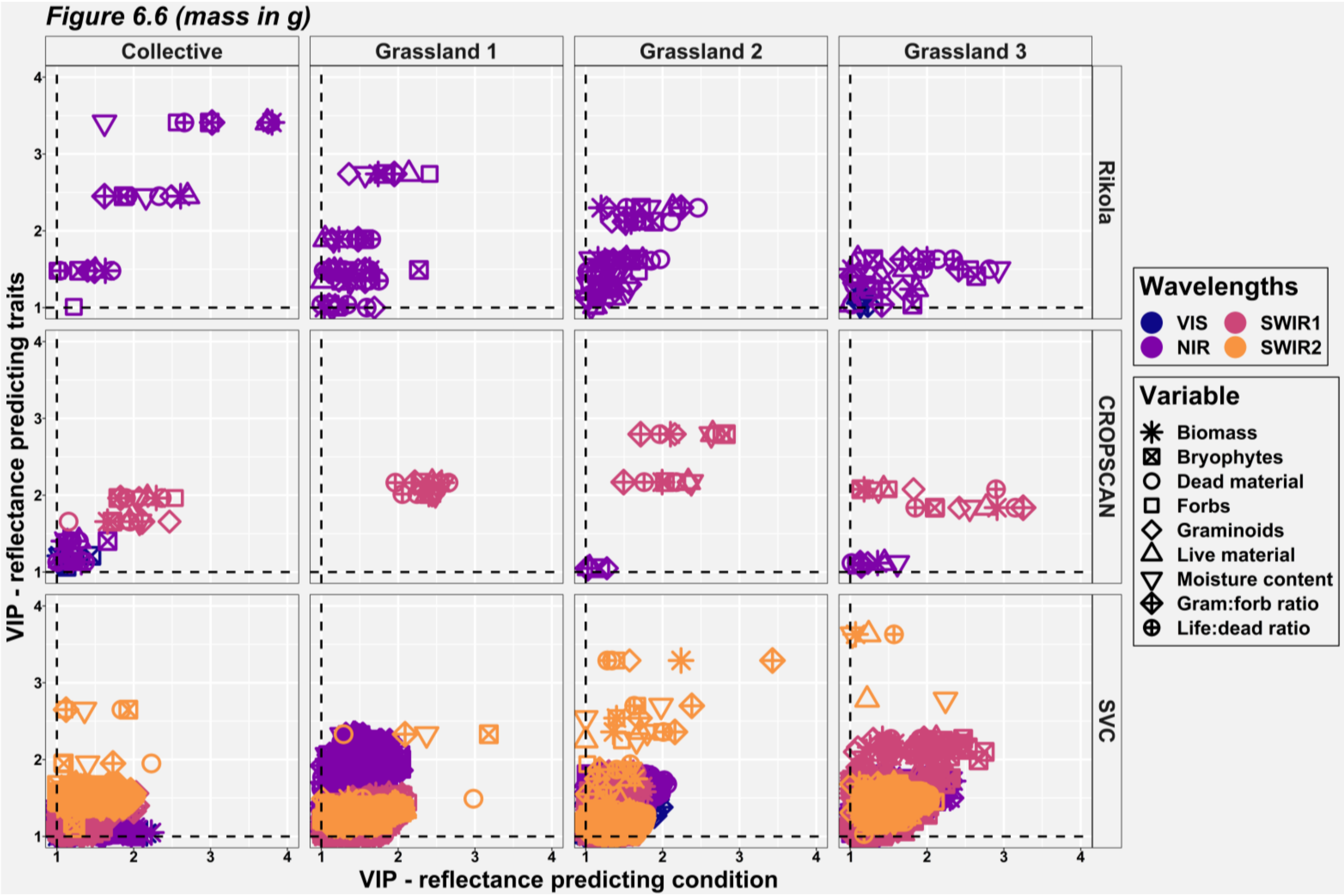
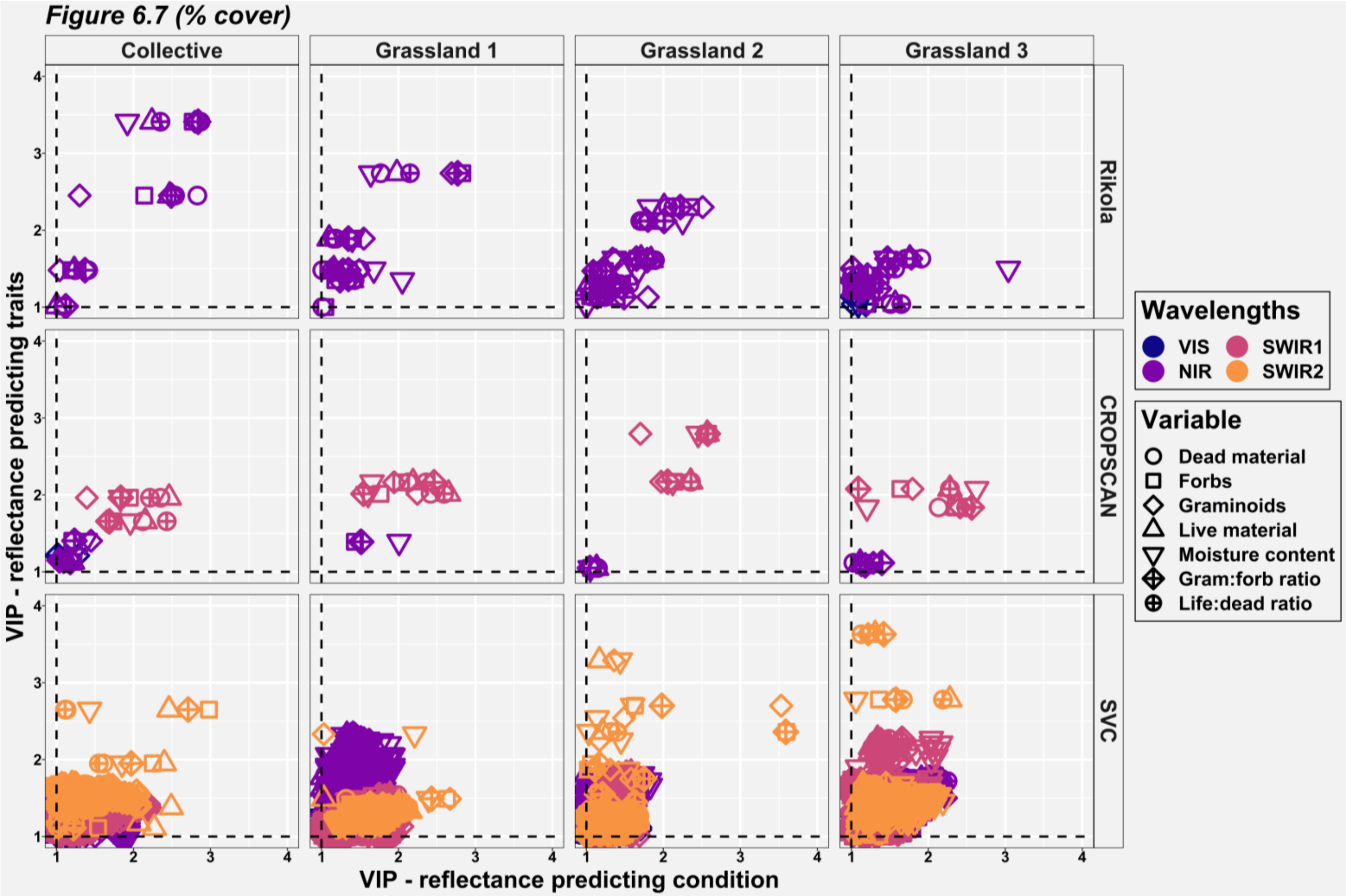



*Figure 6.6: VIP plots showing which regions of spectral data from three different devices and which responses (grassland variables on x axis and CSM-condition on y axis) are most important in the study PLSR models where mass-based grassland variables are used as response data.*

2949 


2950 *Figure 6.7: VIP plots showing which regions of spectral data from three different devices and which responses (grassland variables on x axis*
2951 *and CSM-condition on y axis) are most important in the study PLSRs where % cover-based grassland variables are used as response data.*

## 6.7. Comparison of PLSR models trained with actual data and PLSR models trained with random data

The median values of $R^2$ and nRMSE results presented in Figures 6.2 and 6.3 (referred to as actual models) were compared against the results of 999 further model runs with randomised response variable values (referred to as randomised models) to test the validity of the actual models. The results seen in Figures 6.8 and 6.9 suggest that producing actual or true models that are superior to a randomised model primarily depends on the quantity of data being used, not on the spectral device used to collect the spectral data being used as predictors. Almost all median nRMSE results, and median $R^2$ results for some grassland variables produces actual results that are consistently superior to results found by chance (i.e. from the randomised models), particularly when analyses are carried out on all grasslands collectively (*n* = 30). Only some nRMSE results, and a few $R^2$ results, are consistently better in more than 95% of cases regardless of whether data from all grasslands or single sites are used to train the PLSR models (*n* = 10 or 30).

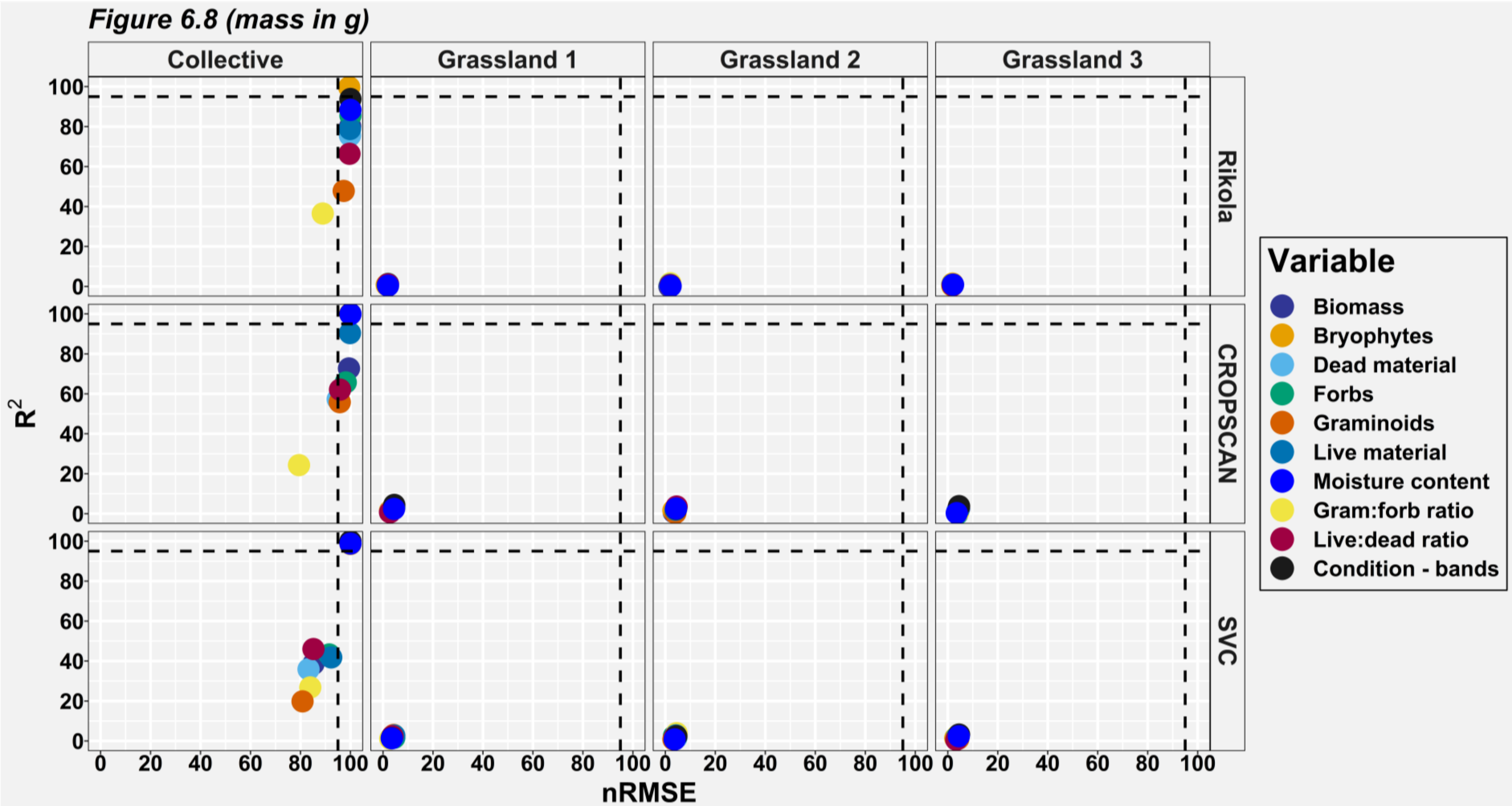
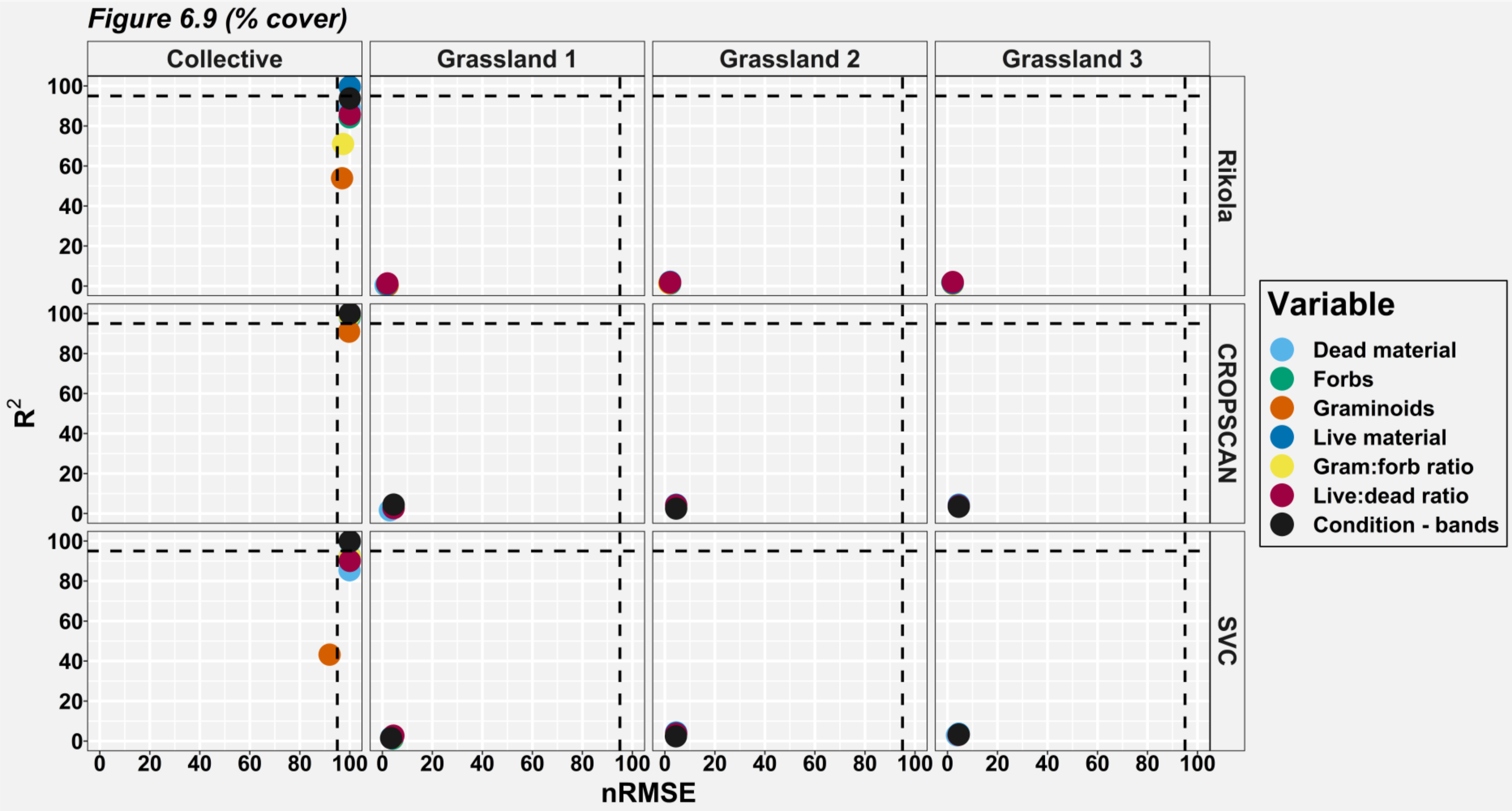



*Figure 6.8: Rankings of the median values of the iterated model runs using actual mass response data and 999 model runs using randomised mass response data, where rankings >95% are considered significant for the actual model fit.*




2971

2972 *Figure 6.9: Rankings of the median values of the iterated model runs using actual % cover response data and iterated model runs using*
2973 *randomised % cover response data, where rankings >95% are considered significant for the actual model fit.*

# Chapter 7 – Discussion

## 7.1. Effectiveness of using PLSR in a RS of grassland condition study

PLSR has been utilised in grassland studies that used a range of RS devices, combinations of spectral data as predictors and grassland condition metrics as either responses or as predictors of other metrics. A PLSR modelling approach has been used in some studies to predict a wide range of biophysical and/or biochemical grassland variables at canopy scale (Capolupo et al. 2015; Schweiger et al. 2017; Wang et al. 2019) or leaf scale (Roelofsen et al. 2014). Other studies have targeted only a few related metrics or solitary metrics such as LAI (Darvishzadeh et al. 2008; Yuan et al. 2016), FAPAR (Sakowska et al. 2016), equivalent water thickness (Li et al. 2008), LDMC (e.g. Ali et al. 2019), nitrogen concentration (Polley et al. 2022; Yuan et al. 2016) plus soil pH and groundwater levels (Roelofsen et al. 2015).

Many model comparison studies have been conducted to ascertain which modelling approach has superior predictive power for any given condition-related grassland variables and PLSR has been utilised in several of these model comparison studies. Linear regression models trained with vegetation indices (VIs) were also commonly included in model comparison studies. Capolupo et al. (2015) found that PLSR had superior performance to four VIs when predicting the quantities of a range of nine structural and biochemical grassland variables on experimental grasslands using drone-acquired hyperspectral imagery. The results of using VIs to predict three structural variables ranged from $R^2$ = 0.3-0.599 but ranged from $R^2$ = 0.63-0.86 when using PLSR. When predicting six biochemical variables, using VIs produced results of $R^2$ = 0.001-0.51 while PLSR results ranged from $R^2$ = 0.21-0.8. Wang et al. (2019) compared the ability of PLSR and Gaussian processes regression (GPR) to predict fifteen different grassland biochemical and structural variables on experimental grasslands using data from the NASA AVIRIS aircraft. Both modelling approaches produced models with moderate to strong predictive power for all variables except lignin and chlorophyll a + b with $R^2$ values > 0.55 (some with $R^2$ values > 0.8). Ali et al. (2019) found that PLSR had superior performance to using eleven different VIs when using Sentinel-2 spectral data to predict LDMC on wetlands ($R^2$ = 0.71) although four of the eleven VIs also produced relatively strong results ($R^2$ = 0.67).

Some model comparison studies have also been conducted at patch level. Sakowska et al. (2016) assessed the performance of using data collected using an Analytical Spectral Device (ASD) set up to automatically collect spectral data across a swath of an experimental grassland, which was resampled to resemble Sentinel-2 data, to investigate the potential of the Sentinel-2 satellite to monitor three different biophysical parameters (CCC, FAPAR, and green FAPAR (GFAPAR)). One aspect of this study was a model comparison between the VIs, MLR and PLSR (where MLR and PLSR models were trained with full spectral data) to predict CCC and GFAPAR. Although PLSR models had superior predictive power for GFAPAR (adjusted $R^2$ = 0.77, 0.78, and 0.82 for VIs, MLR and PLSR respectively), the three modelling approaches had similar predictive power for CCC (adjusted $R^2$ = 0.88, 0.9 and 0.89 for VIs, MLR and PLSR respectively). Darvishzadeh et al. (2008) compared the ability of PLSR and two VIs (NDVI and SAVI) to predict LAI and canopy chlorophyll content (CCC) at patch level on heterogeneous Mediterranean grasslands. Although PLSR produced higher $R^2$ results of 0.69 and 0.74 for LAI and CCC respectively, using VIs also had a moderate to strong predictive power with results of $R^2$ = 0.49-0.64 for LAI and $R^2$ = 0.51-0.69 for CCC. Yuan et al. (2016) used PLSR to predict the quantities of nitrogen concentration and leaf mass per area of two types of crops (sweet corn and snap beans) using different ranges of SVC spectral data as predictors. The results ranged from $R^2$ = 0.8-0.96 (model fit and validation results) depending on the spectral region utilised, with the strongest results either using the full spectral range available for the SVC (450-2400nm) or the 1500-2400nm range. Yuan et al. (2016) claimed that PLSR produced superior results based on a literature review, they did not carry out a comparison study themselves.

Other studies have also used modelling approaches similar to PLSR that have produced models with moderate to strong predictive power, or found that other approaches produced models with stronger predictive power than PLSR. Homolová et al. (2014) compared the ability of VIs, stepwise MLR and PLSR to estimate five different condition-related grassland variables on grasslands that represented a range of grazing regimes. Hyperspectral imagery collected using the aircraft-mounted AISA Dual system were collected for use as model predictors. For four of the five variables (dead material, crude protein content, species diversity and soil carbon content) it was found that stepwise MLR had the strongest predictive power ($R^2$ = 0.6-

0.97) but VIs were strongest for live material ($R^2$ = 0.54). Only the strongest results were presented, so it is not possible to say how much stronger the strongest models were relative to other trained models. Atzberger et al. (2015) compared two statistical modelling methods (predictive equations and VIs, both utilising *in situ* LAI and spectral data) and two radiative transfer models (RTM) inversion methods (one based on look-up-tables and one based on predictive equations) to estimate LAI using hyperspectral imagery collected by an aircraft-mounted HyMap sensor. All methods produced $R^2$ values of 0.75-0.91, but concerns were raised that the accuracy and robustness of the statistical modelling approaches decreases when fewer samples are used for calibration.

# 7.2. The use of mass- or cover-based variables for condition assessment

The primary aim of this research is to assess the link between condition-related grassland variables, plus CSM-condition as defined in this thesis, with grassland spectral reflectance on semi-natural grasslands. As a precursor to achieving this aim, it was deemed necessary to select semi-natural grasslands that represented a spectrum of different grassland types for data collection which was done with an aspect of subjectivity. In other words, grasslands were chosen based on NVC type (based on several semi-quantitative measures) but also several other qualities that remained qualified rather than being converted to a quantity such as grazing intensity. To test whether the chosen grasslands represented a spectrum of significantly differing quantities of the condition-related variables chosen for this thesis, Wilcoxon rank sum tests were conducted on the mass and % cover of data collected on condition-related variables over space and time. The first test was conducted on all seven different grassland types chosen for this thesis. The second and third tests focussed on three chalk grasslands with differing levels of improvement, one of which focussed on the summer season and the other looked at data collected over three seasons.

The exploratory boxplots in Figure 4.2, which used data from all seven grasslands collected during the summer, suggest that the mass of some grassland variables (bryophytes mass, dead material mass and forbs mass) can be used to differentiate between grassland types. The seven grasslands analysed are grasslands that strongly contrast in species, improvement level and grazing intensity. Also, biomass, graminoids mass and moisture content can be used to differentiate some of the seven different grassland types, particularly grasslands 6 and 7 which are a regenerated and a semi-improved grassland on limestone geology. Dead material cover and live:dead ratio cover can also be used to differentiate some grassland types, particularly grassland 5 which is an acid mire grassland. The results suggest that only some of the grassland variables considered in this study are significantly different between grasslands, though some of these results concur with the study of Fliervoet (1987) where biomass (and LAI) were found to be significantly different between different grassland types. When only the less strongly contrasting grasslands with differing levels of improvement located at Parsonage (Grasslands 1-3) are analysed (Figure 6.1), biomass, bryophytes mass, dead material mass, live material mass and moisture content showed significant differences in quantities between some grasslands with differing levels of improvement. The mass of other grassland variables plus all % cover grassland variables showed no significant difference in grassland variable quantities between grasslands. The results suggest that grasslands with differing levels of improvement may not necessarily have significantly different quantities of condition-related grassland variables. Biomass and dead material quantity depends on the species present and grazing/mowing regime (Bai et al., 2001); therefore if the same regime is applied to all grasslands (cow grazing using a similar number of cows confined to that particular grassland) then this could result in these grassland variables not being significantly different between grasslands. It is possible that some forb values plus graminoid and gram:forb ratio values are not significantly different between grasslands, despite Grassland 1 being more species rich. Grasslands 2 and 3 had forb species associated with more improved grasslands such as *Trifolium pratense* (Red Clover) and *Trifolium repens* (White Clover) (JNCC, 2004).

When taking seasonality into consideration (Figure 5.1), no grassland variables for mass or % cover were significantly different between all grasslands and for all three seasons. Some grassland variables were significantly different on one or two grasslands for at least one season and spring is the season where grassland variables are more often significantly different. Mass data were significantly different between grasslands more frequently than % cover data, where many % cover grassland variables were not significantly different to any of the other grasslands. For % cover grassland variables, grasslands were significantly different between more grasslands over three seasons during spring for dead material, live material and graminoids.

The results suggest that the different levels of improvement of the grasslands do not make them considerably different with respect to the grassland variables chosen for this study. One possibility is that it was not the quantities of forb and gram:forb ratio that were different but the forb species present. In other words, while the grasslands were structurally similar, more improved grasslands had forb species associated with these types of grasslands such as red clover and white clover while less improved or unimproved grasslands includes forb species associated with grasslands in better condition (JNCC, 2004; 2006). The structural complexity of grasslands, and how these changes in time, is discussed in Herben et al. (2000). In summary, Herben et al. (2000) explain how the spatial-temporal changes in patterns of species, particularly dominant species over a period of years, results in structural changes described as “fast” when looking at grasslands at a “small” scale but grasslands remain structurally similar over time at a “large” scale (small and large in this context was not defined by the authors, but small seems to refer to patches $<=0.25m^2$ based on referenced literature). This change is driven by a combination of internal and external factors and there are multiple theories behind the dynamics of the changes in species within a grassland over space and time. Species presence as well as abundance can change over time on a given patch, contributing to small-scale structural change

The grasslands at Parsonage Down (Grasslands 1-3) were under-grazed in spring (Hope, S., 2018. pers. comm., 11 July), particularly Grassland 1, which may have contributed to the character of grassland variables being relatively different in spring relative to summer and autumn. In particular, it was observed that a relatively high quantity of dead material existed on the grasslands in spring. A build-up of dead material leading up to data collection in the autumn is also apparent when looking at how the quantities of dead material for each quadrat changes over time. Specific to this thesis, it could be that as the results of the Wilcoxon rank sum tests and the training of PLSR models for spring and autumn were impacted by this build-up of dead material. Although it is believed that dead material was the primary influence in seasonal differences, there are a list of other variables that could have contributed that cannot be tested in this thesis. These variables include seasonal changes in weather, changes in soil nutrients (and potentially pH through fertilisation), differences in grazing regime and differences in aspect and slope (Stevens et al.

2016). The grasslands chosen for this study have the same grazing regime plus the transects were placed where the slope was minimal (0-4$^{o}$) which would have minimised the effect of aspect.

It is possible that collecting data on grasslands that are not considerably different in quantities of condition-related grassland variables had repercussions for PLSR model training. The lack of variation in condition-related grassland variable quantities would have limited the ability to detect changes in condition using trained PLSR models. Alternatively, the lack of variation could be related to the small quantity of samples collected where the full variation of condition-related grassland variables was not fully captured.

# 7.3. Predicting grassland variables and CSM-condition

## 7.3.1. Predicting grassland variables and CSM-condition using spectral data as predictors

To directly address the primary aim of this research, PLSR was used to assess the link between the mass or % cover of condition-related grassland variables plus CSM-condition with grassland spectral reflectance. In general, the results of training PLSR models using data (*n* = 10) from individual grasslands (Figures 4.4, 5.2, 5.3, 6.2, 6.3) showed that most grassland variables can be predicted from reflectance data with $R^2$ values >0.5 and nRMSE values <100. It is possible that overfitting has occurred for results of $R^2$ >0.9, although aspects of the PLSR method should have prevented this (Land et al., 2011). In contrast, when grassland sites are treated collectively (where three, four or seven sites are combined or data collected over three seasons are combined), most of the $R^2$ values of resulting PLSR models mostly drop below 0.5. In other words, predictive models that are site specific appear to be more accurate than those that aim to represent multiple sites. This outcome is entirely expected as grouping data sets is mixing different populations and heightening structural heterogeneity, even though this coincides with an increase in sample information within the context of this thesis (*n* = 30, 40, 70 or 90). When the validity of PLSR models is tested by comparing them with randomised models (Figures 4.8, 5.8, 5.9, 6.8 and 6.9), the results suggest that training PLSR models with 10 quadrats of data (where data collected on one grassland is utilised for model training so *n* = 8) was insufficient to produce a model fit that has significantly stronger $R^2$ and nRMSE values than a randomised model. Though nearly all actual models were superior to randomised models for nRMSE it has been shown that training PLSR models with <20 samples may lead to unreliable models (Goodhue et al., 2012).

When PLSR models were trained with mass data from all three Parsonage grasslands collectively within or across seasons (Figures 5.2 and 5.3), more variables were moderately or strongly predicted in spring or autumn than summer. Conversely, when PLSR models were trained with % cover data, very few variables were predicted moderately or strongly during spring and autumn. When data from all three seasons were utilised to train PLSR models, models with moderate to strong predictive power were produced for particular variables regardless of whether mass or % cover data were used. This suggests that future studies should consider when data is collected as well as which data sets are collected and the quantity of data collected on each grassland. It is possible that the results of using % cover data to train PLSR models results in weaker predictions on grasslands with relatively high quantities of dead material when compared to training models with mass data. Although it has been demonstrated that a high dead material cover affects the spectral signature (Xu et al. 2014; Yang and Guo, 2014), potentially leading to weaker predictive models, this thesis used the same spectral data as predictors in PLSR models trained to predict mass and % cover of condition-related grassland variables. This suggests that changes in spectral signature due to high dead material cover was not the root cause of producing PLSR models with weak predictive power *per se* but could be related to the weak PLSR models trained with % cover from spring and autumn.

A specific variable cannot be recommended for all grasslands and conditions achieving a higher $R^2$ or lower nRMSE depended on the grassland variable, how those data were collected (mass or % cover) and site with no obvious pattern. However, for some grassland variables (Figures 4.5, 5.4, 6.5) the model performance across sites was more consistent (i.e. low $R^2$ and nRMSE CVs). Variables used in model training that were relatively consistent across grasslands, seasons and spectral devices include biomass, bryophytes (mass and % cover), forb cover, moisture content, live:dead ratio cover and CSM-condition. Live material was relatively stable except when using % cover data with data from different spectral devices. Model results for other variables were relatively stable under a specific set of circumstances. For example, model performance for graminoids was relatively stable across seasons on Parsonage grasslands and for dead material mass when using different spectral devices. The inconsistencies in model performance highlighted by the CV results could be due to using an insufficient quantity of data to train some of the statistical models, in other words there is inconsistency because some PLSR models were trained with only 10 quadrats of data. Overall, there appears to be less consistency in results when using mass data relative to using % cover data for some grassland variables. This could be due to a lack of spatial coverage of sampling when collecting mass data, which meant that the complexity of the grasslands was not effectively captured.

In broad terms, previous RS condition studies have used multispectral or hyperspectral RS data in combination with *in situ* data and models for the assessment of vegetation condition (e.g. Psomas et al., 2011). Few studies where grassland variables were predicted by RS methods included the use of grassland constituent mass and no studies have defined a comparable CSM-condition metric or used grassland variable data to predict a CSM-condition metric. Guo et al. (2005) used OLS regression and correlation analyses to link condition-related biophysical grassland variables with NDVI and LAI on a spatially heterogeneous prairie. Using regression and LAI values as predictors, patch level ($1m^2$) dry biomass was predicted with a $R^2$ value of 0.598 and moisture content with a $R^2$ value of 0.903. Furthermore, correlation coefficient values were between r = 0.7-0.8 when correlating LAI with biomass, graminoids and forbs and when correlating NDVI with moisture content. Correlation between LAI and moisture content was 0.903. Psomas et al. (2011) investigated the strength of the relationship between above ground biomass and spectral reflectance at patch level using multiple linear regression and VIs, where they found that feeding 2-4 specific spectral bands into an MLS regression produced the strongest predictions of biomass ($R^2$ = 0.77-0.86) and the $R^2$ results for all VIs were <0.6. Chen et al. (2009) also tested the strength of the relationship between biomass and spectral data at patch level on spatially heterogeneous grasslands, using VIs as predictors in PLSR. This study collected data at different angles to better capture grassland structure and shadowing, but dead material was removed from destructive samples after spectral readings had been taken in spite of studies (Asner, 1998; Asner et al., 2000; Xu et al., 2014) that show that dead material influences the spectral signature. If dead material % cover was low as suggested but not quantified, this may have not strongly influenced the spectral signature of quadrats (Yang and Guo, 2014). The highest $R^2$ values (0.52-0.54) were achieved by using PLSR and single narrow band reflectance or first-order derivative reflectance. Yang and Guo (2014) assessed the strength of the relationship between dead material % cover and a range of VIs using linear and non-linear regressions, where almost all of the results of using different VIs and different regressions were $R^2$ = 0.53-0.56, where data were collected on patches with dead material % cover of 45-56%. Davidson et al. (2006) compared OLS regression models trained to predict moisture content (absolute and relative) using different VIs and ranges of spectral data directly used as predictors. Using spectral data ranges and some VIs as predictors appeared to train models with relatively strong predictive power ($R^2$ = 0.7-0.8). However, the $R^2$ values of these two studies could be erroneous as multicollinearity effects were not addressed.

When predicting biomass on a range of different grassland types (Chapter 4); of 16 model runs that used data from Grasslands 1-3 (Parsonage), five model runs produced results of $R^2$ >0.5 and nRMSE <100 ($R^2$= 0.54-0.59 and nRMSE = 55.6-76.8). Of 20 model runs for Grasslands 4-7 (Ingleborough), all had values of $R^2$ >0.5 and all but two had nRMSE values of <100 ($R^2$= 0.56-0.94 and nRMSE = 46.8-110.2) with the results of the collective analyses having a range of $R^2$= 0.56-0.67 and nRMSE = 67.7-75.4. It is not clear why biomass was predicted more effectively on some grasslands, or combination of grasslands, as there does not appear to be a link with grassland structure (taking structural complexity and grazing regime into consideration) or level of improvement and biomass prediction strength. Furthermore, there did not appear to be a clear link with a relative lack or abundance of a particular grassland variable and biomass prediction. Although weaker PLSR models generally seem to be trained with data collected on grasslands with a relatively high % cover of dead material and low % cover of forbs, this pattern is not strictly the case as Grassland 7 does not fit this pattern. Grassland 7 does not appear to be more heavily grazed than Grassland 6 or more improved than Grasslands 2 or 3.

When dead material was predicted in this study; training PLSR models with mass data from both locations ($R^2$= 0.57-0.60 and nRMSE = 74.9-75.9) or Ingleborough (Grasslands 4-7, $R^2$= 0.50-0.88 and nRMSE = 45.7-88.9) almost always produced moderate to strong predictions. Relatively few PLSR models produced moderate to strong predictions when trained with % cover data from both locations or from Grasslands 4-7. When PLSR models were trained with data from Grasslands 1-3, the only moderate to strong prediction ($R^2$ >0.5) that did not seem to be dubious ($R^2$ >0.9) was produced by a model trained with % cover data from all three grasslands collectively ($R^2$= 0.53 and nRMSE = 47.3). It is not clear why destructive sampling captured dead material more effectively on Ingleborough grasslands compared to Parsonage grasslands. Grassland 2 (Parsonage) plus Grasslands 4 and 5 (Ingleborough) have a dead material cover of 0-25% but the other grasslands have a lower dead material cover of 0-8%, suggesting that there is a relatively high variance in dead material within each location. This suggests that increased variance in % cover of dead material does not positively or negatively impact the predictive power of the PLSR models.

When moisture content was predicted in this study; most of the predictions were weak ($R^2 < 0.5$) but stronger predictions ($R^2 > 0.5$) were produced by analysing Parsonage or Ingleborough grasslands collectively and for Grasslands 1, 4 and 6. There appears to be a pattern where the models with $R^2$ values >0.5 were trained with data either from all grasslands within one location or from alkaline grasslands. It is not clear why this should be the case. Although all three Parsonage grasslands had a similar mean soil moisture (0.104-0.111$m^3$ water/$m^3$ soil) and three of four Ingleborough grasslands also had a similar mean soil moisture (0.358-0.409$m^3$ water/$m^3$ soil), Grassland 5 is an acid mire grassland and had a relatively high mean soil moisture (0.787$m^3$ water/$m^3$ soil). Other soil data were not collected to verify whether these soil moisture readings were affected by high organic content, which may be considered useful as increased organic content may make a soil more poorly draining. Also, Grasslands 3 (Parsonage), 4 and 5 (Ingleborough) had a relatively high variance in moisture content. Furthermore, training a PLSR model with Parsonage or Ingleborough grasslands collectively produces moderately strong models, but training a model with data from both locations produces a weak PLSR model.

When predicting biomass within or across different seasons (Chapter 5), of the 32 model runs using either FULL or VNIR spectral data, 19 model runs produced PLSR models with $R^2$ => 0.5 and nRMSE <100, with a range of $R^2$ = 0.5-0.91 and nRMSE = 45.5-98.1. The strongest six of these PLSR models, and the most PLSR models with $R^2$ >0.5 of these 32 models, are for Grassland 3 with more of these PLSR models produced using autumn data. It is not clear why most of the strongest models were trained on data collected in autumn as the quantities of grassland variables for the summer season were generally similar (but with increased dead material cover in autumn relative to summer). Although canopy structure is considered to be primarily responsible for canopy level reflectance characteristics, biochemical variables were not considered in this study and this could have influenced the results to an unquantified extent (Cole et al. 2014). It seems clearer that a reduced amount of biomass and an increased amount of dead material would have affected the training of PLSR models to predict biomass in spring.

Of 64 model runs for dead material (either mass or % cover responses and either FULL or VNIR predictors), 25 model runs produced PLSR models with $R^2$ => 0.5 and nRMSE <100 with a range of $R^2$ = 0.5-0.97 and nRMSE = 25.5-77.6. Of these model runs, 19 used % cover data. Also, analysing data from all seasons or spring produced most of the PLSR models with $R^2$ => 0.5. Asner et al. (2000) shows how seasonal changes in dead material influence the factors (i.e. grassland variables) that affect variability in spectral reflectance. A high dead material content had a relatively stronger influence on the visible part of the spectrum (40-60% of variance) but also on the NIR part of the spectrum (20-40% of variance). This may explain why most of the PLSR models with moderate or high predicting power were trained at least in part using spectral data from spring, when the dead material cover on the grasslands was particularly high (up to 70% cover). The influence of high dead material cover on the spectral signature may also have reduced the models' predictive power for other grassland variables (Asner et al. (2000); Xu et al. (2014); Yang and Guo (2014)).

When PLSR models were run with moisture content as response data, most of the predictions were weak ($R^2$<0.5) but stronger predictions ($R^2$>0.5) were produced by analysing data from Parsonage grasslands collectively (Grasslands 1-3) for summer and for Grassland 2 for some seasons (spring, summer and when using data from all three seasons) plus Grassland 3 for spring. The results of comparing these models to models trained on randomised data (Figure 5.8) suggest that the models trained on data from individual grasslands are unreliable because of the low sample size. One possibility for stronger predictions of moisture content during the summer is that the sampling strategy better captured the variation in moisture content by chance. Variance for moisture content data is 2.05 for summer compared to 1.27 and 0.69 for spring and autumn respectively. Another reason could be the increased dead material cover during spring, and to a lesser extent, autumn having an impact on the spectral data which were then used as predictors in the models. Asner (1998) conducted an aircraft RS study on a range of semi-arid grasslands, shrublands and transition zones (succeeding from grasslands to shrublands) in the Brazilian Cerrado to link vegetation variables with the variation of wavelengths in the 400-2500nm spectral region. The results suggest that on grasslands; the dominant biophysical factors on the variation of reflectance in the 400-2500nm spectral region were soil reflectance, litter reflectance and transmittance (at the leaf level) and the fractional cover of grass canopies. Soil reflectance was the most dominant factor across the whole 400-2500nm spectral region, likely because of relatively sparse vegetation cover, but litter was the next dominant factor in the VNIR part of the spectrum. Although there was minimal soil cover on the grasslands chosen for this thesis, it could be that dead material and canopy structure had a relatively strong influence on the spectral signature which partly explains the results seen in Chapter 5.

When comparing the prediction of grassland variables using data from different spectral devices (Chapter 6); models trained to predict bryophytes, moisture content and CSM-condition (but not for moisture content when using Rikola data) were the models with moderate to strong predictive power. When using % cover data; live material and CSM-condition were moderately to strongly predicted by models trained with spectral data from any three of the spectral devices used in this study. Models trained with CROPSCAN or SVC data also had moderate to strong predictive power for forb cover and gram:forb ratio cover. Models trained with CROPSCAN data also had moderate to strong predictive power for dead material cover and live:dead ratio cover.

Yao et al. (2013) showed that models with stronger predicting power can be produced when trained using ASD spectral as predictors compared to using CROPSCAN spectral data as predictors (possibly due to an increased range or quantity of bands) although this study predicted nitrogen quantity on croplands. This thesis suggests that similarly good results can be produced from using CROPSCAN or SVC data, but it is possible that using the methods proposed in this thesis does not fully utilise the additional spectral data gained from using the SVC the way that some authors (e.g. Psomas et al., 2011) may have done.

In general; different grasslands, spectral data or seasons did not produce a markedly different number of PLSR models with $R^2$ => 0.5 when spectral data were used to predict grassland variables and CSM-condition and when grassland variables were used to predict CSM-condition. An exception is that most of the superior PLSR models trained to predict CSM-condition with spectral data were trained using data collected in summer. When grassland variables were used to predict CSM-condition, most of the superior PLSR models were trained using % cover data.

There are numerous potential reasons for the lack of consistency in predicting grassland condition-related variables across different grasslands and seasons. It is possible that a holistic study (Homolová et al., 2014; Lausch et al. 2018), or at least a wider-ranging study that captured data on more variables would have highlighted condition-related variables that could be more consistently predicted with a moderate to high level of accuracy and precision. It has also been suggested that time and resource restrictions prevent this (Lausch et al. 2018) and therefore the variables considered to be more promising based on the literature review were chosen. Alternatively, it could be that an approach that better accounted for at least some of the limitations pointed out in Section 7.7 would have led to more consistent results. For example, an approach where more data could be collected within time and cost constraints or a modelling approach that could better capture the variation in the condition-related variables chosen or could better predict the lowest and highest variable values (Chen et al. 2009; Psomas et al. 2011).

### 7.3.2. Predicting CSM-condition using grassland variables

When using grassland variable data collected over a wider range of grasslands to predict condition (Chapter 4), the results suggest that some grassland variables are more important predictors of CSM-condition across different types of grasslands than others. For predicting CSM-condition across different types of grasslands, live:dead ratio using mass or % cover appears to be a particular important variable with other relatively important variables including forbs cover, graminoids cover, gram:forb ratio mass and gram:bryo ratio mass.

When using grassland variable data collected over multiple seasons to predict condition (Chapter 5), the results suggest that which grassland variables are most important depend on whether mass or % cover data are used; biomass, gram:forb ratio mass, live:dead ratio mass and moisture content when using mass data but dead material cover, forbs cover, graminoids cover, live material cover and live:dead ratio cover when using % cover data. Focusing on data collected at Parsonage during the summer forbs cover, graminoids cover and live:dead ratio cover were important for predicting CSM-condition when using % cover data whilst gram:forb ratio mass and live:dead ratio mass were important when using mass data although there were slight differences between grasslands. When using mass data; biomass was important when using data from Grassland 1 and gram:forb ratio mass was not important for Grassland 3 whilst graminoids cover was not important to Grassland 2 when using % cover data. As all of the grassland variables used in this thesis are considered to be related to condition, it is possible that these results are related to how well each grassland variable is captured by a particular method of data collection (i.e. % cover or mass) although it is possible that changes in vegetation across seasons and particularly the changes in dead material quantities had an impact on the results. Another possible reason for some of the aforementioned grassland variables being considered significant is that they were used, either directly or indirectly, as criteria to calculate CSM-condition. For example, dead material cover was a criterion for establishing CSM-condition for some grasslands which would relate to the grassland variable live:dead ratio cover.

## 7.4. Extrapolating predicted grassland variables

The practical purpose of the research in this thesis is to provide land managers with a methods to monitor grassland condition on semi-natural grasslands with improved time-efficiency and spatial-temporal coverage. To achieve this, the results of PLSR models trained with CROPSCAN data were extrapolated from patch to field level (Figure 6.4). For extrapolation, an emphasis was placed on trained PLSR models that had been trained with grasslands from all grasslands collectively as other results in this thesis (Figures 4.8, 5.8, 5.9, 6.8 and 6.9) suggested that PLSR models trained using data from individual grasslands (*n* = 10) may not be able to consistently improve on models trained with random data. Most of the PLSR models trained with collective grassland data had weak predictive power ($R^2$ <0.5 and/or nRMSE >100) though most of the PLSR models trained using % cover and CROPSCAN data sets were at least of moderate predictive power ($R^2$ >0.5 and/or nRMSE <100). Although extrapolated predicted values have been presented in Figure 6.4, it is not clear how accurate these predictions are as it is not possible to externally validate the results aside from the leave-one-out cross-validation (LOO-CV) approach used to derive nRMSE and the calculation of the PRESS statistic (used in this thesis to choose optimum number of components for model training) due to the small sample size of the data sets. External validation of the results using a data set completely separate from the one used to train the models would have been a more robust external validation approach (Ramspek et al. 2021). An example of a study which took this approach is Schweiger et al. (2017).

Furthermore, it was observed from the drone data and the projections of the predicted values from the PLSR models that the pattern of grassland variable predicted values appears to follow the spatial pattern of the varying illumination levels of the imagery. In other words, a higher illumination value for that image pixel meant a higher grassland variable value predicted by the PLSR models. This suggests that issues caused by within *and* between image illumination have not been solved in this study and an effective solution does not currently exist to the knowledge of the author. This means that these results are not reliable as it would be necessary to equalise illumination variation both within and between images before analysis to prevent this issue for occurring. A potential solution to this issue is the use of VIs for model training, but multiple studies (e.g. Arroyo-Mora et al. 2021) have discussed the negative impact of variable illumination conditions on derived vegetation indices. Despite this, some authors have also discussed potential solutions for combining image processing with VIs selected specifically because of the reduced impact of variable illumination conditions on their calculation relative to some alternative methods such as those discussed in this thesis. For example, utilising reference panels as a means of correcting UAV imagery can improve the consistency of image illumination, but any approach that assumes relatively stable illumination during the flight, i.e. makes one calibration before or after the flight, can still lead to erroneous results. On the one hand, the use of spectral devices that collect repeated measurements of upwelling and downwelling radiation could provide solutions to variable illumination. Alternatively, authors may instead use an approach such as automated multiscale Retinex correction before calculating VIs to improve the validity of the results (Wang et al. 2023). Arroyo-Mora et al. (2021) found that an atmospheric correction approach should be chosen based on the conditions during the flight, i.e. using the MODTRAN-5 based radiative transfer model achieves better results in high direct irradiance conditions while an Empirical Line Model (ELM) approach is more applicable under more diffuse and variable irradiance conditions. They also found that the calculation of NDWI was less impacted by variable irradiance conditions than other VIs such as NDVI. Souza et al. (2021) found that calculations of NDVI, NDWI and the red edge inflection point were relatively stable compared to other VIs when comparing calculations derived from imagery collected in sunny conditions and imagery collected in cloudy conditions. Wang S et al. (2019) proposed using Tucker tensor decomposition to remove the effects of cloud shadowing as an added step to improving the reliability of images affected by cloudy conditions.

When the predicted values from the PLSR models trained with CROPSCAN spectral data were projected, the trend in the predicted values between grasslands appeared to be as expected. The regenerated calcareous grassland (Grassland 1, NVC = CG2) had an increased quantity of bryophyte mass, live material % cover, forbs % cover and CSM-condition plus decreased dead material % cover and gram:forb ratio (derived from % cover data) compared to the two semi-improved grasslands. These trends are associated with grasslands of a better condition although an increase in forbs % cover can be associated with more improved (lower condition) grasslands due to an increase % cover of species such as Red Clover (*Trifolium pratense*) and White Clover (*Trifolium repens*) (JNCC, 2004; 2006). As explained earlier, it was not possible to externally validate the results using a data set separate from model training therefore the only validation of the results was achieved using the leave-one-out cross-validation (LOO-CV) approach used to derive nRMSE.

To the knowledge of the author, the only comparable literature currently available focused on prediction of biomass or grassland variables related to biomass such as grass height on experimental grasslands. Capolupo et al. (2015) used PLSR models trained using UAV-acquired spectral data as predictors of structural grassland variables. Their study was conducted on experimental grasslands over two seasons at field level. Using one season of data; wet biomass, height and dry biomass produced $R^2$ results of 0.72, 0.7 and 0.63 respectively. These results improved to >0.8 when two seasons of data were analysed collectively. Lussem et al. (2019) used OLS regression to estimate dry biomass on experimental grasslands that had a range of fertilisation (improvement) levels. Three VIs were calculated using spectral data collected with two UAV-mounted devices. The Plant Pigment Ratio Index was considered to produce more accurate predictions ($R^2$= 0.7) than the NDVI ($R^2$ = 0.63) and Normalized Green Red Difference Index (NGRDI) with $R^2$ = 0.57 when these indices were used as predictors in the OLS regression. Although LOO-CV was applied, only absolute RMSE values were provided so the model error is not clear and it is not possible to compare model performance between models using $R^2$ and nRMSE results. As part of a wider study, Viljanen et al. (2018) used estimated grass height, VIs and spectral data collected with a UAV as separate or combined predictors of biomass on experimental fields; in this case to train OLS regression and random forest models using data collected on four different dates in June. The $R^2$ and nRMSE results for each date ranged from 0.82-0.93. Again, it is not clear how model overfitting was prevented although it is unlikely to have happened if models were trained with only a few features. Michez et al. (2019) also estimated canopy height (this time using LiDAR data) then used either these estimated canopy height values, spectral data collected using a UAV, or a combination of the two to train four different types of models to predict biomass. Spectral data were either utilised in models as reflectance values or as VIs. The best performing model had a $R^2$ value of 0.49 where the model was trained using a combination of estimated canopy height, reflectance values and VIs. Like the previous study, data sets were collected within one month (May) and therefore grassland variability over the growing season was not captured.

Théau et al. (2021) estimated biomass and vegetation cover on experimental pasture plots using a range of methods; structure from motion (SfM) and non-linear regression to predict biomass plus a classification (cluster) analysis to estimate vegetation cover. A range of VIs, calculated by extracting spectral data collected with a drone, were used as predictors in the latter two analyses. Linear regression between estimated biomass using the SfM approach and observed biomass produced $R^2$ values of 0.93 and 0.94 for fresh and dry biomass respectively with nRMSE values <10%, although only 12 samples ($n$ = 12) were used in this analysis plus it is not clear how the analysis was carried out and therefore how overfitting was prevented. For heavily-grazed grasslands where a structure from motion (SfM) approach is ineffective, the results of using green NDVI (GNDVI) as a predictor produced the most accurate predictions of estimating biomass with $R^2$ values of 0.80 and 0.60 and nRMSE values of 24% and 29% for fresh and dry biomass respectively. Grüner et al. (2019) estimated canopy height using a SfM approach then estimated dry biomass with the aid of estimated canopy height using reduced major axis regression on experimental grasslands. The strength of the predictions of biomass ranged from $R^2$ = 0.46-0.87 subject to the treatment that a given experimental grassland had received, which was attributed to differences in the variability of the canopy structure of each grassland. It is not clear if confounding variables have some responsibility for the variation in results. Furthermore, this approach would possibly be flawed if used to estimate biomass on heavily grazed grasslands, but it is not clear if this is the case.

This study did not use grass height as a grassland variable (although it played a minor role in determining CSM-condition) and the PLSR models trained using data from all Parsonage grasslands collectively presented in this study had weak predictive power for biomass. On the other hand, the PLSR models had strong predictive power ($R^2$=> 0.7) for live material % cover. All of the aforementioned papers used experimental grasslands as study sites and did not make available the data sets collected on these grasslands. It is possible that the standard linear regression approaches produced particularly strong results because the grassland data collected to train the models were uniform because the grasslands studied by the aforementioned authors (e.g. Viljanen et al. (2018)) were structurally homogeneous. In practical terms, the models would be overfitted as they would have no predicting power for more structurally heterogeneous grasslands. For this reason, it is thought that inferences made by authors such as Lussem et al. (2019) that biomass predictions on experimental grasslands can be transferred to other grasslands are likely to be false. Addressing this would require experimental grasslands to replicate the structural heterogeneity (both within and between grasslands) observed on semi-natural grasslands such as the grasslands selected for this thesis.

A similar situation may have occurred with the mass-based observations in this study. Despite collecting data on more structurally heterogeneous grasslands, the models appeared to lack the ability to predict the highest mass values such as where tussocks were located. One reason could be that the data collection approach did not successfully capture the structural heterogeneity both within and between the grasslands in three dimensional space, a consequence of collecting a relatively small data set. Alternatively, a change in some grassland variable values did not result in a sufficient change in the spectral signature for the trained model to predict values that are much higher than most of the other grassland variable values. The inability of the models to predict much higher values could also be a result of using a linear regression approach.

## 7.5. Choice of spectral bands

One goal of this thesis is to explore which spectral reflectance bands, and related to this which radiometry instruments and regions of the EM spectrum, would be most useful in training PLSR models with strong predictive power. This thesis used VIP to understand which model predictors were most important for the predictive power of the trained models. Spectral data from each device was autoscaled prior to analysis to remove the possibility of the VIP results being positively biased towards the NIR part of the spectrum. In general for all three devices used in this thesis, the VIP results (Figures 4.6, 5.5, 5.6, 6.6 and 6.7) suggest that the bands in the upper part of their spectral range (upper NIR and SWIR bands) were most important for predicting grassland variables. To use the CROPSCAN as an example; the most significant bands for predicting a wide range of grassland variables across different locations, seasons and when using different data types are the SWIR bands and upper NIR bands (760-1640nm) along with the red edge (647nm) and blue band (470nm) to a more limited extent. The importance of the upper NIR and SWIR bands, regardless of the device used, is highlighted by looking at how many wavelengths in these regions was considered an important predictor (Figures 6.6 and 6.7) for all of the PLSR models trained (Figures 6.2 and 6.3) for this particular study (Chapter 6).

For the CROPSCAN (collects data on 16 wavelengths); the SWIR1 range produced nearly twice as many VIP values >1 (125) than the NIR range (77) and approximately six times more than using the VIS part of the spectrum (22) when predicting grassland variables, all of the VIP values >2 are in the SWIR1 range. For the Rikola camera (collects data on 30 wavelengths); the NIR range produced approximately six times more VIP values >1 (672) than using the VIS region of the spectrum (121) when predicting grassland variables. For the SVC (collects data on 1249 wavelengths); the NIR and SWIR1 regions of the spectrum (8989 and 9753 respectively) produced more VIP values >1 than the VIS or SWIR2 regions of the spectrum (4407 and 5183 respectively).

These results suggest that the aforementioned bands better capture and/or are more sensitive to changes in CSM-condition and the condition-based grassland variables used in this study regardless of grassland, season or device. These results agree with some studies (e.g. Chen et al., 2009; Polley et al. 2020) and disagree with others (e.g. Capolupo et al., 2015) although the studies where the results disagree did not use instruments that collect data on the SWIR part of the spectrum. Despite this, it could be that the upper NIR bands being strong predictors of grassland variables and condition generally explains why the results of using FULL and VNIR data are similar. Furthermore, the CROPSCAN only collects data on two bands in the SWIR region of the EM spectrum.

When considering the results of the VIP analysis (where specific bands in the VIS and red edge regions of the spectrum were also deemed important), one possibility is that these results are influenced by grassland canopy spectral reflectance being strongly influenced by chlorophyll and water absorption (Knipling, 1970). The VIP results could also be explained by previous studies which show the importance of NIR and SWIR bands in predicting grassland variables (Asner (1998); Chen et al.

(2009); Roelofsen et al. (2015)). Chen et al. (2009) used spectral data ranging from 400-1100nm in their analyses and used a band importance index (BII) to highlight which bands were most important in predicting biomass. The BII results suggested that parts of the NIR range and blue range of the spectrum were the most important ranges of bands for predicting biomass. These findings were reiterated when Pearson's correlation was used to test the strength of correlation between the reflectance at each wavelength and aboveground biomass. The results from this study match their results quite closely, except this study used two bands from the SWIR part of the spectrum which were also found to be important. Capolupo et al. (2015) found that VIS (450–545 nm) was most important in predicting some grassland variables including fresh biomass and grass height, but their study also used a more limited part of the spectrum (450-950nm). Using simulated spectral signatures, Xu et al. (2014) found that increased bare soil cover increased reflectance along the whole spectral signature whilst increased dead material cover decreased NIR reflectance and increased SWIR reflectance. Roelofsen et al. (2015) related changes in the NIR parts of the spectral signature to leaf orientation and LAI plus the SWIR part of the spectrum to water content in agreement with findings by Asner (1998).

One aspect of this thesis is to try to understand how important it is to utilise SWIR data when training predictive models. In Chapters 4 and 5, models were trained with two different ranges of spectral data; VNIR (visible and NIR data) and FULL (VNIR plus two SWIR wavelengths). In Chapter 4, models trained with VNIR data produced higher $R^2$ and lower nRMSE results for most grassland variables when analysing grasslands from both locations or Ingleborough grasslands collectively. Full spectrum data (FULL) produced stronger predictions for most grassland variables and for condition when analysing Parsonage grasslands collectively. When the results of analysing individual grasslands are compared, whether using full spectrum or VNIR data produces higher $R^2$ values is dependent on the grassland type and grassland variable. For biomass, live material or dead material $R^2$ results (mass or % cover); full spectrum results are almost always weaker than using VNIR. Overall, the ratio between occasions when each produced stronger results was almost 1:1 in favour of using VNIR data. Both spectral data ranges produced a similar number of significant results ($R^2$ >0.5 and nRMSE <100).

One of the aims of the thesis addressed in Chapter 6 was to assess whether spectral data from different devices can accurately predict CSM-condition or the mass or %

cover of condition-related grassland variables and to compare the performance of the PLSR models trained using data from these different spectral devices. Of 192 model runs (Figures 6.6 and 6.7), 76 were considered moderate to strong on the basis that the results had $R^2$ values => 0.5 and nRMSE <100; 35 model runs for CROPSCAN, 16 for the Rikola camera and 25 for the SVC. Some of these models (49) had $R^2$ values => 0.7; 20 for CROPSCAN, 14 for the Rikola camera and 15 for the SVC. When comparing how many PLSR models made moderate to strong predictions of grassland variables using spectral data from each device, no one variable stands out as producing many more significant results than the others. All grassland variables except biomass, bryophytes and dead material produced 10-13 significant results each (mass and % cover). Biomass and bryophytes were used in half as many model runs (only mass data) and produced 3 and 5 significant results respectively. All 5 of the significant results for dead material were the result of using % cover data. Using % cover data produced 52 significant results whilst using mass data produced 24 significant results. For the CROPSCAN, SVC and Rikola camera; the ratio of significant results when using % cover data is 23:16:13 and when using mass data it is 12:9:3. It is possible that relatively few models trained with Rikola spectral data had moderate to strong predictive power because the SWIR region of the spectrum is relatively sensitive to water content which correlates strongly with chlorophyll content (and, in turn, biomass) in other studies (Sakowska et al., 2016).

## 7.6. Practical implications of RS condition monitoring of grasslands

Unlike most comparable studies which are conducted on experimental or relatively structurally homogeneous grasslands and in clear sky conditions, the RS studies of grassland condition in this thesis were carried out on spatially heterogeneous grasslands (within and between grasslands) and in changeable weather conditions which can introduce error and uncertainty into RS studies. For example, Harzé et al. (2016) found that specific leaf area (SLA), leaf dead matter content (LDMC), and plant height are characterized by considerable intra-population variability (SLA: 72–95%, LDMC: 78–100% and vegetative height: 70–94% of the variability of grassland variables) as a result of within-site environmental heterogeneity including variables such as soil depth and slope. It is thought that this variability plus variation in aspects of the grazing regime of each grassland, particularly grazing intensity (Bai et al., 2001) could have made it more difficult to link spectral data to grassland variables and condition on the semi-natural grasslands chosen for this study. Furthermore, on the mire grassland included in this study; tussocks, sinkholes and shrubs complicated the collection of good quality RS data because spectral data can be influenced by topography and canopy structure. Also, the calcareous grasslands of Ingleborough NNR included a limestone pavement where outcropping rocks affected the spectral signature. Although the aforementioned within-grassland variability of some grassland characteristics and geographic features may have increased model error in predicting the grassland variables included in this study, these features of semi-natural grasslands are not taken into consideration in studies conducted on experimental grasslands (e.g. Capolupo et al., 2015), meaning their methods may not be viable on semi-natural grasslands. In contrast to many other RS studies on grassland condition, the mass of grassland variables (graminoids, forbs, bryophytes and dead material in particular) were used as responses in regression analyses. These grassland variables can be linked to condition for the reasons explained in Chapter 2, in particular Sections 2.1 and 2.3.6.

The results of this study have implications for future studies that try to predict condition-related grassland variables using a RS methods. If models need to be calibrated to individual grasslands (particularly grasslands that are as spatially heterogeneous as the ones studied) to produce stronger predictions, more *in situ* data is required to capture the within-grassland variability in grassland variables and related grassland canopy structure. Many of the models with values of $R^2$ >0.7 were trained using data from individual grasslands ($n$=10 in this thesis), suggesting that site specific studies are more reliable. Comparing these results to the results of randomised models suggests that training statistical models with insufficient data lead to unreliable results even if the study is site specific (Goodhue et al., 2012). Therefore, the results of this study suggest that collecting sufficient data to train the models is critical and a sufficient quantity in this thesis was deemed to be 30 quadrats. Receiving relatively high $R^2$ and low nRMSE results can be deceptive as these same models may not be able to consistently beat randomised models or deliver reproducible results, which also demonstrates the importance of model testing. In addition, it is also important to collect a sufficient quantity of data to allow for validation of the results using a data set separate from the data set used to train the models. The increased number of moderately strong PLSR models produced using data from all grasslands collectively, relative to Chapter 4 which included grasslands from Ingleborough NNR, suggests that using data from different grasslands may have a reduced impact on model strength if all of the grasslands are structurally similar. There are many variables other than canopy structure that influence the spectral signature and were not taken into consideration in this study such as biochemical variables. A study where a larger quantity of samples are collected on each grassland may confirm whether site specific studies produce superior results to studying multiple grasslands. Furthermore, using % cover or mass data seems to capture different condition-based grassland variables more effectively although % cover data can be collected more time-efficiently.

It also seems necessary to use relatively high spatial resolution satellite or drone data that includes the capture of data on at least a couple of SWIR wavelengths to capture the spatial structural heterogeneity of target grasslands when comparing the predictive power of PLSR models trained with CROPSCAN data compared to models trained with Rikola data. The most advanced VNIR cameras mounted on <20kg drones currently available collect data on a 500-900nm range with a spatial resolution of <1m (6cm for the Rikola camera). The results of the PLSR and VIP analyses suggest that predicting grassland variables using this range of spectral data is viable but the strength of grassland variable prediction is dependent on grassland type, grassland variable and how the variable is captured (mass or % cover). Despite this, the results suggest that devices that collected spectral data on SWIR wavelengths (e.g. SVC), even if it is only two wavelengths (e.g. CROPSCAN) trained more models with a moderate to strong predictive power relative to using Rikola data. Considerations need to be made around collecting imagery with UAVs as within and between image illumination levels can have a detrimental impact on the viability of any results gained from using the spectral data from these images as predictors in models. The timing of the flight needs to be as close to the time of highest sun as possible to minimise within and between image illumination variability. The vignetting effect (reduction in illumination at the periphery of the image) also needs to be considered as it will contribute to within image illumination variability (Kordecki et al., 2016). A contributing factor to this issue may have been that this thesis chose the PLSR modelling approach, which can be sensitive to issues related to the viewing angle of the spectral device and the sun as well as surface property differences such as canopy structure (Li et al. 2016).

# 7.7. Study limitations

This study directly attempted to address issues around monitoring the condition of semi-natural grasslands which had practical implications for the robustness of the results from this work. As so many hypotheses were tested at once, the results may have been affected by the multiple testing hypothesis and the “look-elsewhere” effect. Although steps were taken to ensure that the results of this study are reproducible (making it unlikely that the “look-elsewhere” effect is happening), training such a large number of PLSR models has complicated making inferences from the results. Furthermore, PLSR models cannot accommodate a fixed-effect which refers to instances where all the values of the response variable are the same. This prevented PLSR models being trained to predict “bare ground” and “graminoid:bryophyte ratio” for Parsonage grasslands (Grasslands 1-3). Using PLSR as a statistical modelling approach seemed to underestimate the largest grassland variable values and overestimate the smallest grassland variable values (as seen in Psomas et al. (2011) and Chen et al. (2009) respectively), but whether using a non-linear regression approach *per se* would have produced superior results is debatable (Yang and Guo, 2014). One possibility for the above limitations is the variation in spectra that can occur even when many of the variables of a target remain the same (e.g. Price, 1994) which can occur because of spatial and temporal variability in illumination, the problems of which would be exacerbated when using an insufficient quantity of training data in the statistical models. Some of the spectral data collected in spring were incorrectly calibrated and were corrected using spectral data collected at a separate site (see Section 3.4.3.1). It is believed that these corrected data were of sufficient quality for analysis, but it is possible that there was a minor impact on the accuracy and precision of models trained with these data. Data collected with an Analytical Spectral Device (ASD) at Ingleborough NNR was not viable as a result of the highly changeable weather conditions and cloud patterns. Weather conditions also prevented triplicate data collection with the CROPSCAN on all Ingleborough grasslands except the acid mire grassland plus the collection of spectral data at Ingleborough NNR during spring and autumn. Although the results of this study suggest that forbs can be predicted by spectral data with significant accuracy and precision if grasslands are analysed individually, only the species count was able to determine which species of forb existed in a target area. This may be an issue as some forb species are positive indicators while others are negative indicators of condition (JNCC, 2004; 2006). This could be inferred from the species abundance data in this study, but these data were only collected on quadrats during the spring period at Ingleborough NNR and the summer period at Parsonage NNR and species abundance on a given patch can change over time (Herben et al., 2000) therefore this is another limitation. CSM-condition was derived from CSM criteria where multiple data sets including species abundance and % cover grassland variables were used as inputs for the criteria. When % cover grassland variables were used as predictors of CSM-condition, there may have been positive bias as % cover "dead material" and "forbs" were also used for a few of the CSM criteria that CSM-condition was derived from. Furthermore, CSM-condition was calculated using criteria that were weighted equally in the calculation. It is acknowledged that the criteria weights used to calculate CSM-condition could be relaxed or refined and this should be further investigated to establish the optimum weightings of each criterion.

The results of using the mass or % cover of grassland variables to demonstrate that the grasslands in this study are significantly different in character due to differing levels of fertilisation mostly suggested that this was not the case, but it is unclear if the methods used in this study were ineffective as Hollberg and Schellberg (2017) suggested that different intensities of fertilisation can be distinguished using VIs. Collecting % cover data of bryophytes was limited as they grow beneath graminoid and forb species. Also, some quadrats in spring had dead material cover values that were considered high (50-75% for quadrats 1-8 and 35-60% for seven quadrats on Grassland 3) which may have led to increased within-site variability of grassland variables and spectral signatures (Yang and Guo, 2014). The amount of error that may have been introduced by these factors is unknown but the total error for each model run has been quantified using nRMSE. Changing quadrat locations each season introduced spatial-variation to a temporal study which may have complicated the interpretation of the results. This was unavoidable as spectral data had to be collected on quadrats unaffected by destructive sampling as this sampling would have altered the canopy structure and therefore affected spectral data collection (Gitelson et al. 2019). Furthermore, the CSM guidelines suggested that 4m$^2$ quadrats should be used for assessing M19 grasslands but this study used 1m$^2$ quadrats. Finally, this study was also affected by major limitations specific to the extrapolation of the results from PLSR models trained with Rikola spectral data. Although the vignetting effect was addressed to an extent by removing a portion of the image peripheries, this study did not effectively solve the detrimental effect that within and between illumination variation can have on the accuracy of predicted grassland variable values. Furthermore, the predicted grassland variable values extrapolated to field level have not been independently verified against a separate data set to assess the accuracy of the extrapolated results for PLSR models trained with Rikola or CROPSCAN spectral data.

Studies using the same approach as this paper should be conducted on other spatially heterogeneous grasslands and collect a greater quantity of data to confirm that the results would be consistent regardless of the target grassland. Alternatively, a study that is better suited to capturing then mining spatial-temporal data should also be completed to determine if seasonal data would increase the predictive power of regression analyses on grassland variables and CSM-condition.

# 7.8. Potential research opportunities

There are several directions that future research could take in relation to this thesis. There is already a trend towards the increased use of UAVs as remote sensing platforms. If the use of RS data collected with a UAV is to truly become viable, issues related to between and within variances in image illumination would need to be solved. Solving this issue could lead to grassland condition studies on semi-natural grasslands at field level becoming viable. This could coincide with advancements in UAV-mounted instruments, for example they could collect hyperspectral data on a wider range of the EM spectrum or become more economically accessible. As more very-high spatial resolution satellites are launched and their imagery becomes more commonplace, it is possible that grassland condition monitoring at field level will become financially viable but whether this is scientifically possible may depend on which wavelengths data are collected. Hyperspectral satellite imagery with a higher spatial and spectral resolution, for example from EnMap, could also become more available for grassland condition studies in future. Whether hyperspectral satellite imagery can be utilised may depend on the cost of the imagery and the cost of acquiring sufficient computing power.

Regarding machine learning techniques, a model comparison study that includes further exploration of Bayesian (e.g. Zhao et al. 2013), kriging and neural network (NN) techniques could lead to more accurate models although a larger data set may be required to train accurate models (Li et al. 2016). For example, Li et al. (2016) found that regression kriging and random forests residuals kriging predicted LAI more accurately than PLSR, random forests or artificial neural networks. Furthermore, using neural networks may be an effective way to overcome issues related to differences in illumination between and within multi- or hyperspectral images collected with a UAV.  The neural network may produce reliable results without the necessity of image (histogram) equalisation subject to a sufficient amount of spectral data being utilised as training data and taken from different images to capture the changes in illumination (Thomas, T. pers. comm. 1st December 2020.

# Chapter 8 - Conclusion

This thesis assessed whether remote sensing techniques could be used to ascertain the condition, in the context of ecosystem services, of different types of grasslands by predicting condition-related grassland variables with a sufficient level of accuracy. This research is considered important as it could provide more time- and cost-effective approach to grassland monitoring, enabling superior spatial-temporal coverage and more timely intervention of conserving degrading grasslands. Previous studies had been conducted to address issues within this line of research, but these studies were generally limited by not directly tackling the issues around the remote sensing of grassland condition on working semi-natural grasslands. Finding a working solution to establishing the condition of semi-natural grasslands was considered most beneficial to land managers who may adopt this approach as a more cost- and -time efficient approach to condition monitoring with the added benefit of better spatial coverage than traditional monitoring techniques.

This assessment was conducted by training PLSR models using spectral data collected with hand-held devices or by UAV as predictors and using the mass or % cover of condition-related grassland variables plus CSM-condition as responses. Grassland variables were also used as predictors of CSM-condition. The results suggest that it is possible to use these methods to accurately estimate some of the grassland variables chosen by this study subject to some caveats. The results suggested that, despite PLSR being suggested as a correct approach for use with small data sets and to avoid model overfitting, it is still possible to train models that seem to have moderate to strong predictive power but are actually unreliable if an insufficient quantity of data are used. More specifically, the results suggest that most of the PLSR models with moderate to strong predictive power in this thesis are not reliable if they are trained with data from only one grassland ($n$ = 10). A sufficient amount of data to train PLSR models so that the results were considered reliable was considered to be at least 30 quadrats ($n$ = 30). It is possible that collecting larger data sets on each grassland would have solved this issue, but data collection was limited by time and resources and therefore this is not clearly demonstrated in this thesis. Despite these limitations; it was possible to train PLSR models to predict some grassland variables to a moderate to high level of accuracy for some grasslands and seasons.

This has implications for other similar studies which may have assumed their results were robust without using an effective external validation technique. There are also implications for land managers who are interested in implementing RS techniques to monitor the condition of grasslands as it would be necessary to collect a sufficient amount of data to train models with reliable results and to externally validate the results of extrapolated models. This suggests that collecting and separating a sufficient number of grass samples to establish the mass of grassland variables may not be practical but could lead to models trained to accurately predict some condition-related variables that would not be possible when using % cover data. The grasslands and time of year could also be factors when trying to accurately predict condition-related variables as the results of this thesis suggest that none of the grassland variables chosen for this thesis could be consistently predicted with reasonable accuracy across grasslands and seasons. The results of this thesis also suggest that choosing a spectral device that collects data on the SWIR part of the spectrum could help train more accurate models, but this is not crucial.

A number of recommendations are suggested based on the findings of this thesis. The methods used in Chapter 6 to predict grassland variables at field level should include a data set separate from model training to externally validate the predicted values from extrapolated models. These proposed methods, with an external validation approach included, should be tested with an increased amount of response data (i.e. the mass or % cover of grassland variables) and across seasons to test the optimal amount of data and best seasons to collect data for training the most accurate models. If the limitations to using imagery collected by a UAV cannot be overcome (for example, by removing illumination differences within and between images), using a UAV-mounted spectrometer that collects patch level spectral data (i.e. comparable to a CROPSCAN) on many patches over an entire field may be a more suitable device for the prediction of grassland variables at field level. This opens up possibilities for training PLSR models and other types of models making a model comparison study using drone data possible. For example, some studies have used Bayesian techniques or neural networks to determine grassland condition.

The final recommendations and considerations are for land managers contemplating adopting these methods for monitoring grasslands. Land managers would need to decide whether it is practical to collect and separate a sufficient number of grass samples to ensure the robustness of the PLSR models when trying to predict the mass of a given variable. Collecting % cover data on grassland variables is considerably more time-efficient but has its own set of limitations as specified in Chapter 7. When collecting spectral data; considerations need to be made around the spatial and spectral range of any device used, plus the weather conditions though clear sky weather conditions does not guarantee stable illumination. In short, the methods in this thesis offer a more cost- and time-effective solution to monitoring grassland condition but any land manager who implements the methods in this thesis would have to take the aforementioned points into consideration to increase the likelihood of training models with an acceptable predictive power.

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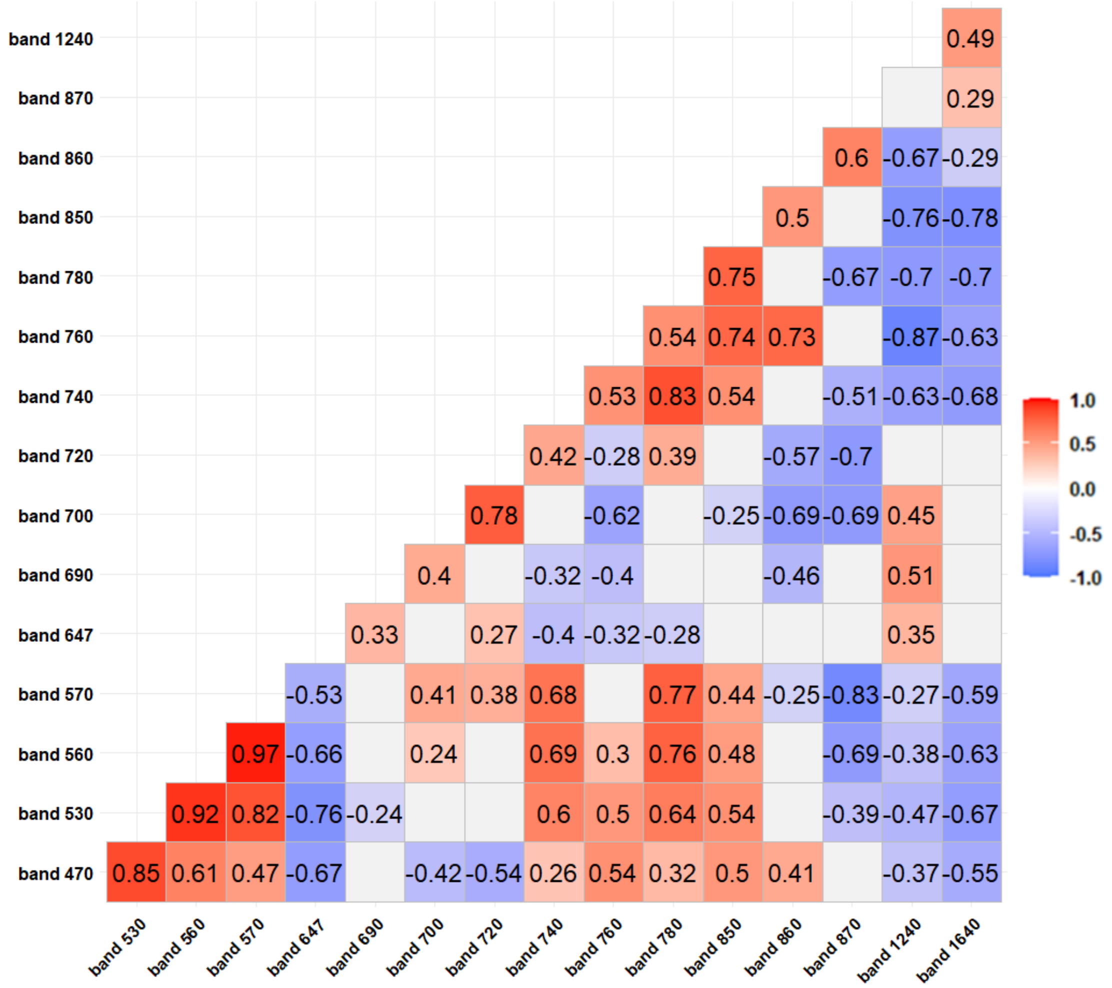
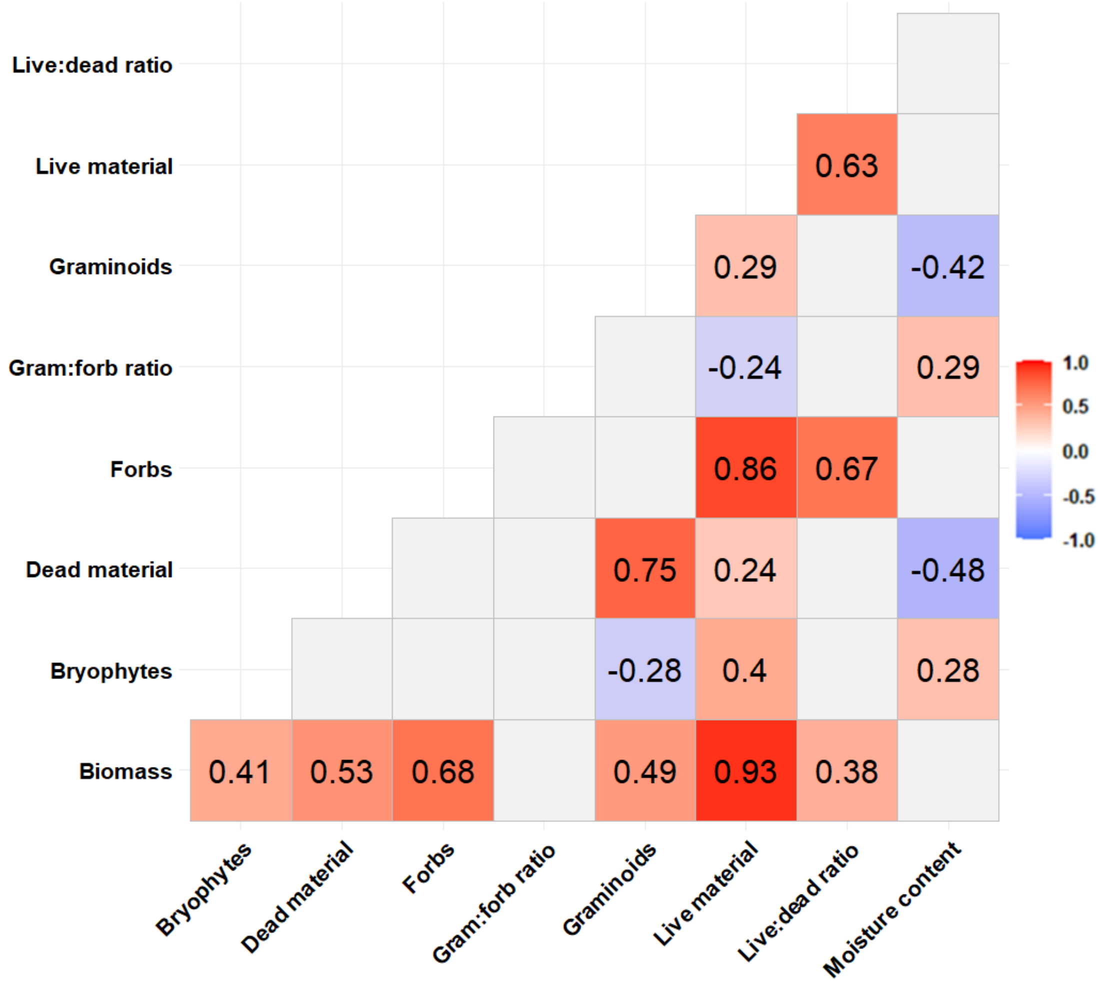
# Appendix

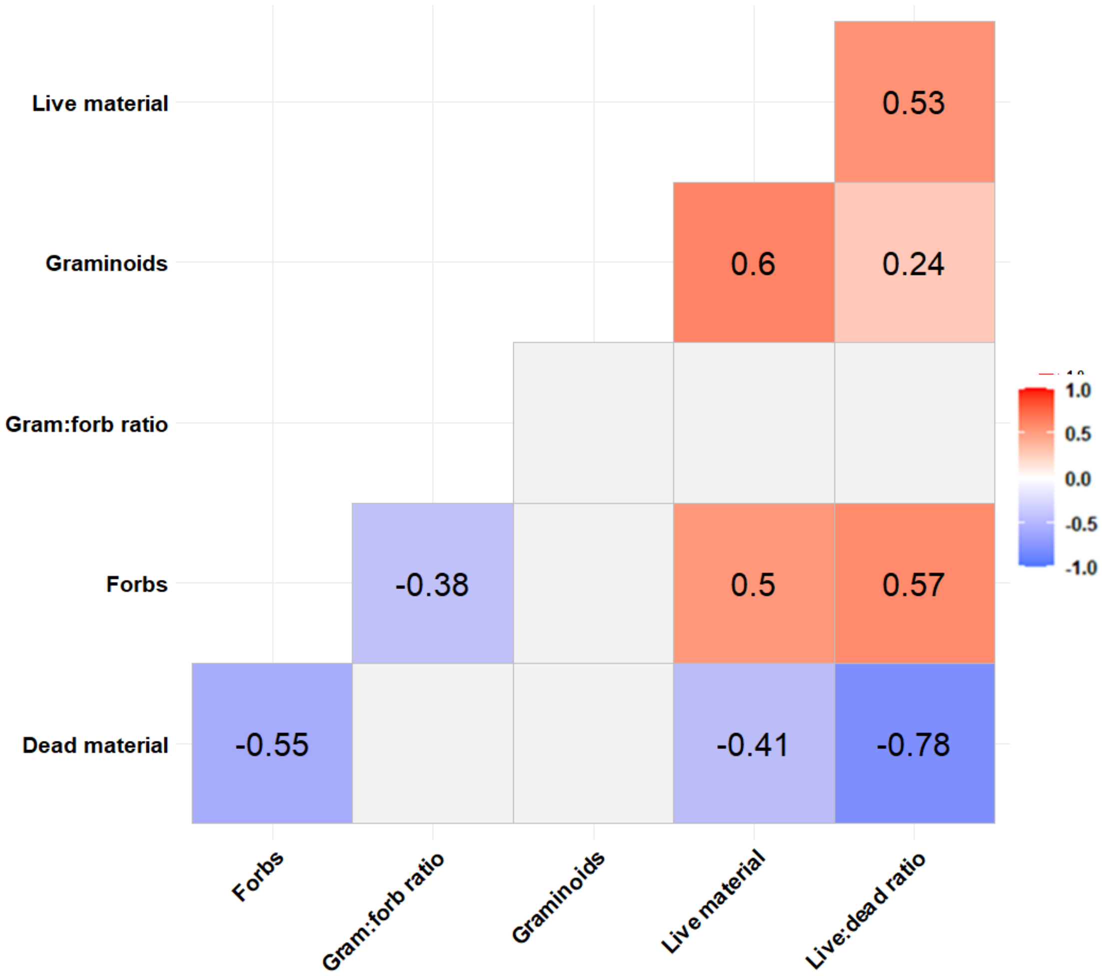
## Correlation matrices



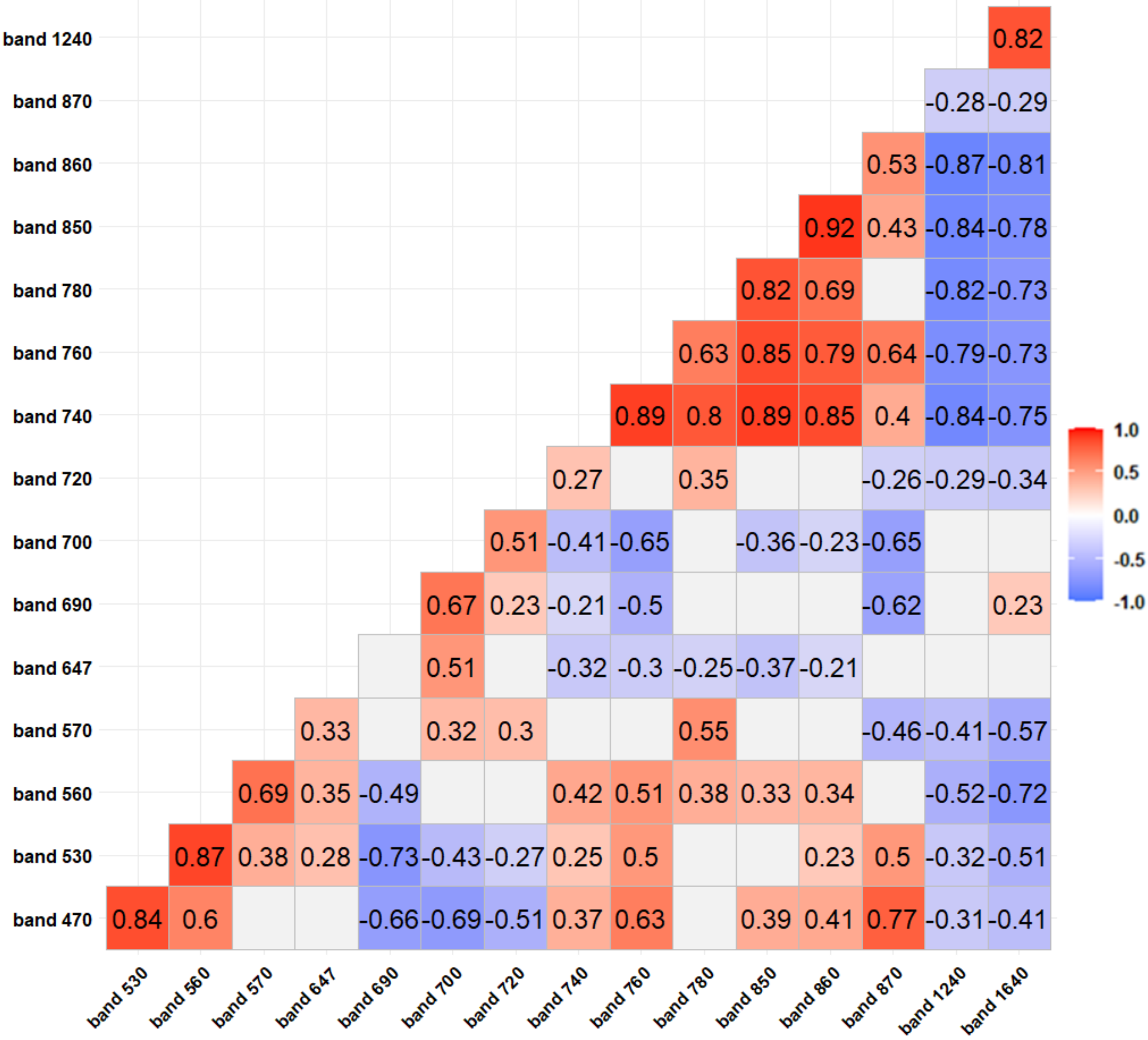


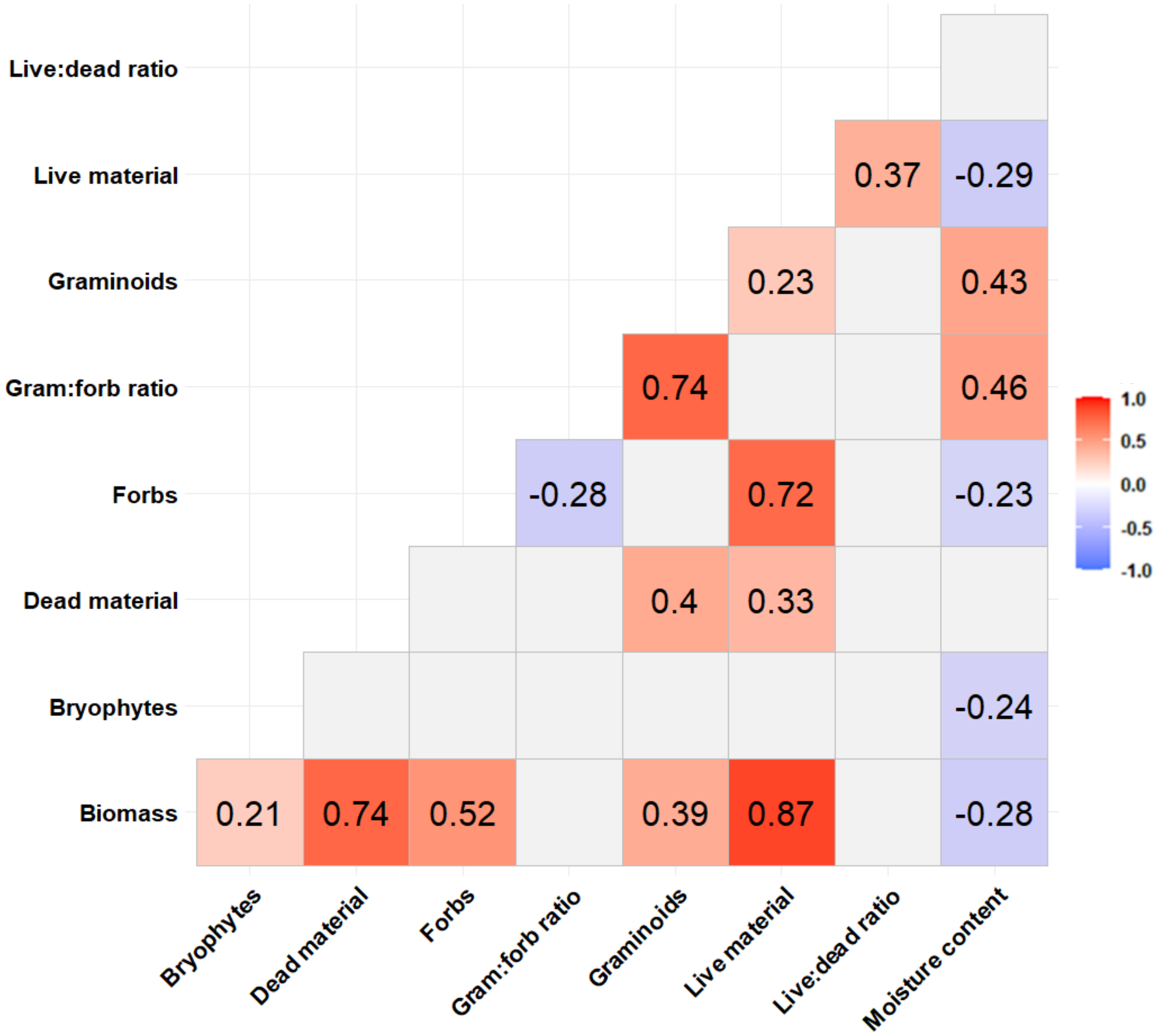
Live:dead ratio
Live material
Graminoids
Gram:forb ratio
Forbs
Dead material
Bryophytes
Biomass
0.63
0.29
-0.42
-0.24
0.29
0.86
0.67
0.75
0.24
-0.48
-0.28
0.4
0.28
0.41
0.53
0.68
0.49
0.93
0.38
1.0
0.5
0.0
-0.5
-1.0
Bryophytes
Dead material
Forbs
Gram:forb ratio
Graminoids
Live material
Live:dead ratio
Moisture content

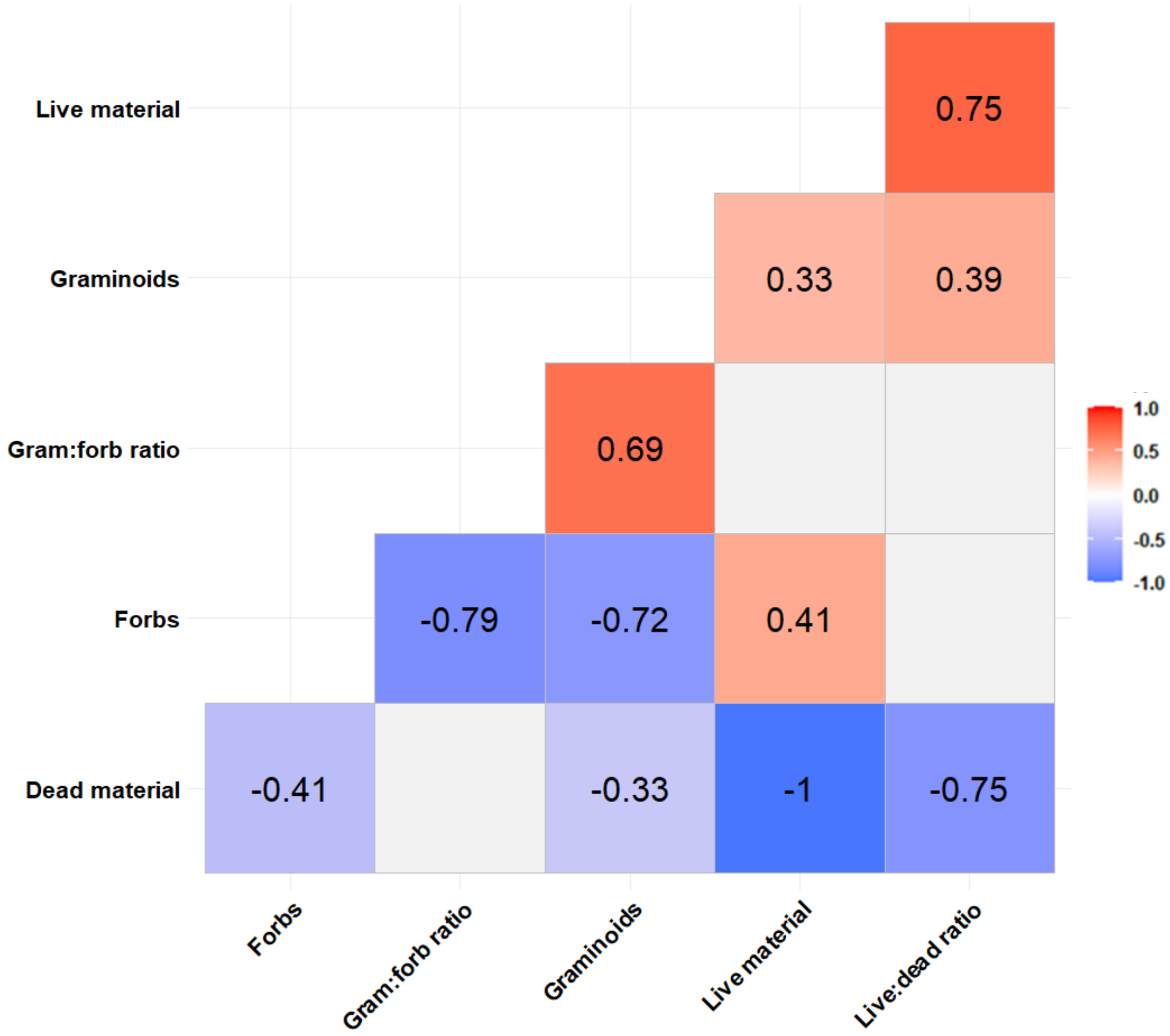

4709




*Appendix Figure 1: Correlation matrices between predictors used in PLSR modelling a) spectral bands, b) mass-based grassland variables and c) % cover-based grassland variables. Correlation coefficients that are not statistically significant (p > 0.05) are not included. The data used to for analysis were collected across seven grasslands during the summer season (n=70). The correlation matrix for the spectral bands from the CROPSCAN (Appendix Figure 1a) indicated statistically significant strong correlations between bands within each of the VIS (390-700nm) and NIR (701-870nm) regions of the spectrum. There are also significant strong negative correlations between NIR bands and SWIR bands (1240 and 1640nm). When using mass-based grassland variables (Appendix Figure 1b), live material mass was strongly correlated with biomass and forbs mass. When using % cover-based variables (Appendix Figure 1c), dead material cover was negatively correlated with live:dead ratio cover with a value of -0.78.*

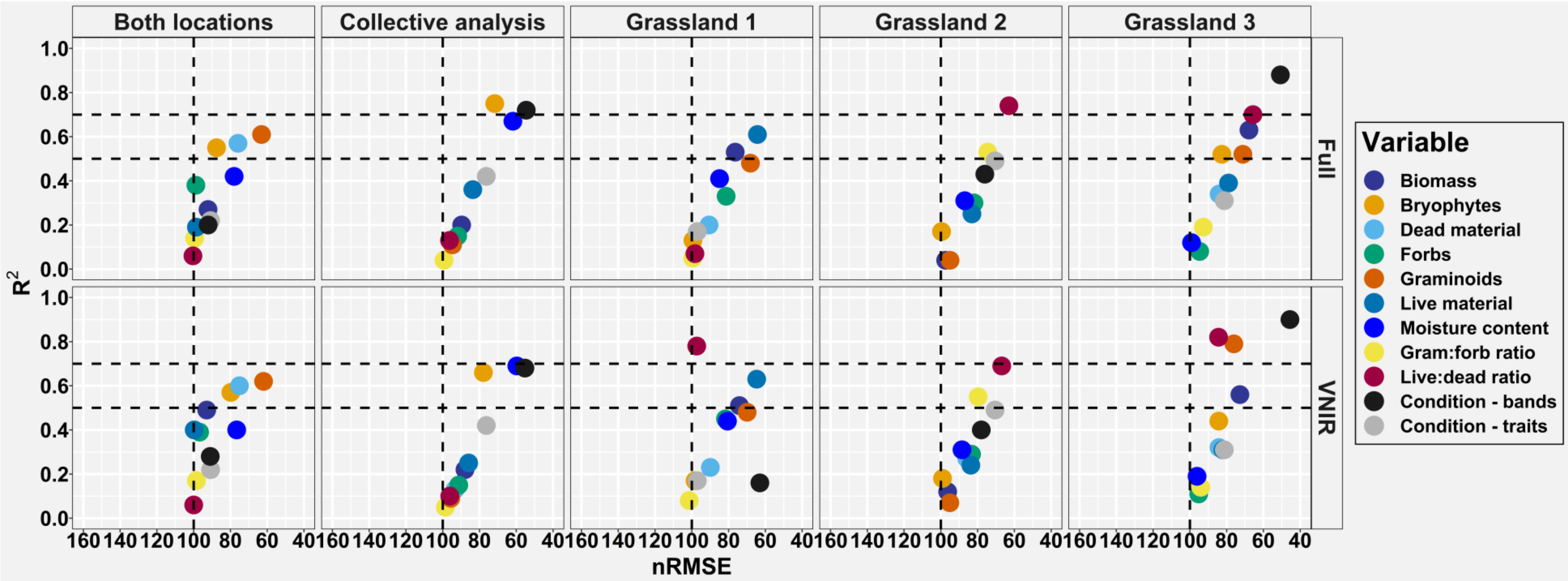

band 1240
band 870
band 860
band 850
band 780
band 760
band 740
band 720
band 700
band 690
band 647
band 570
band 560
band 530
band 470
band 530
band 560
band 570
band 647
band 690
band 700
band 720
band 740
band 760
band 780
band 850
band 860
band 870
band 1240
band 1640
1.0
0.5
0.0
-0.5
-1.0


Live:dead ratio
Live material
Graminoids
Gram:forb ratio
Forbs
Dead material
Bryophytes
Biomass
0.37
-0.29
0.23
0.43
0.74
0.46
-0.28
0.72
-0.23
0.4
0.33
-0.24
0.21
0.74
0.52
0.39
0.87
-0.28
Bryophytes
Dead material
Forbs
Gram:forb ratio
Graminoids
Live material
Live:dead ratio
Moisture content
1.0
0.5
0.0
-0.5
-1.0



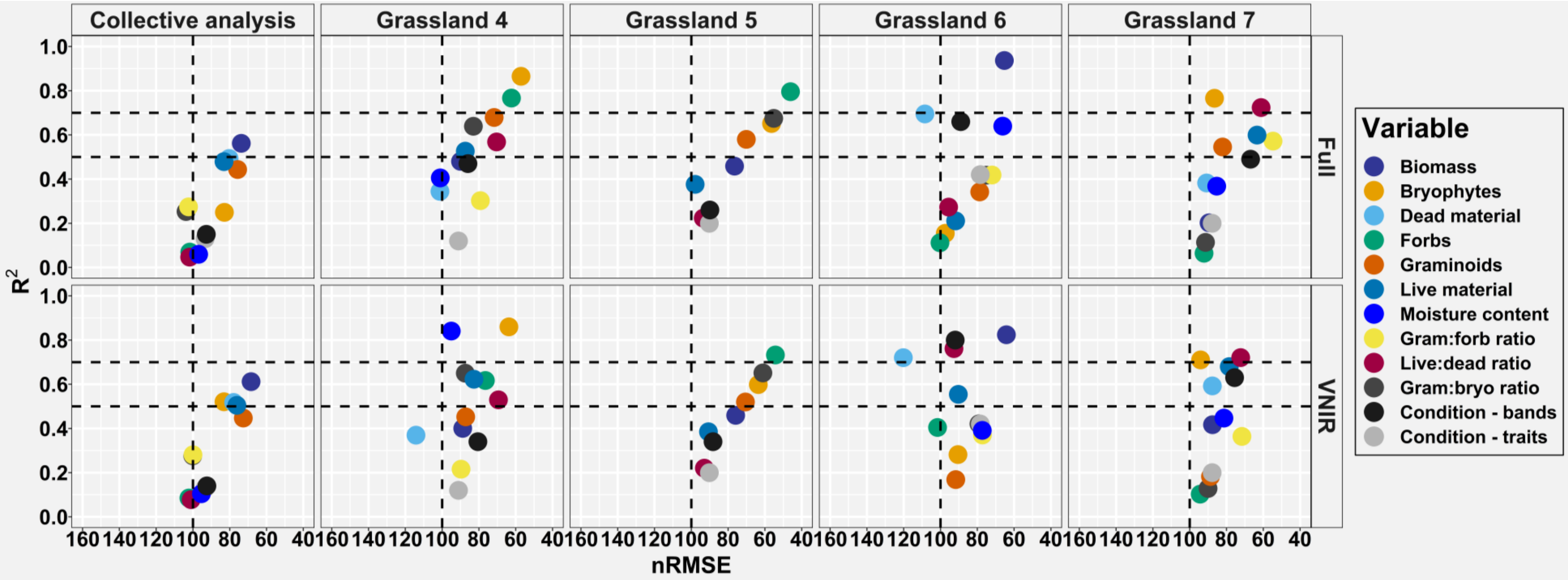

*Appendix Figure 2: Correlation matrices between predictors used in PLSR modelling a) spectral bands, b) mass-based grassland variables and c) % cover-based grassland variables. Correlation coefficients that are not statistically significant (p > 0.05) are blanked out. The correlation matrix for the spectral bands from the CROPSCAN (Appendix Figure 2a) emulated those of Appendix Figure 2a; there were statistically significant strong correlations between bands within the VIS and NIR regions of the spectrum and there are also significant negative correlations between some NIR and SWIR bands. When using grassland variables; the only significant r values were between biomass and live material when using mass-based variables (Appendix Figure 2b), and live material and dead material when using cover-based variables (Appendix Figure 2c).*

4743 ## Chapter 4 full results



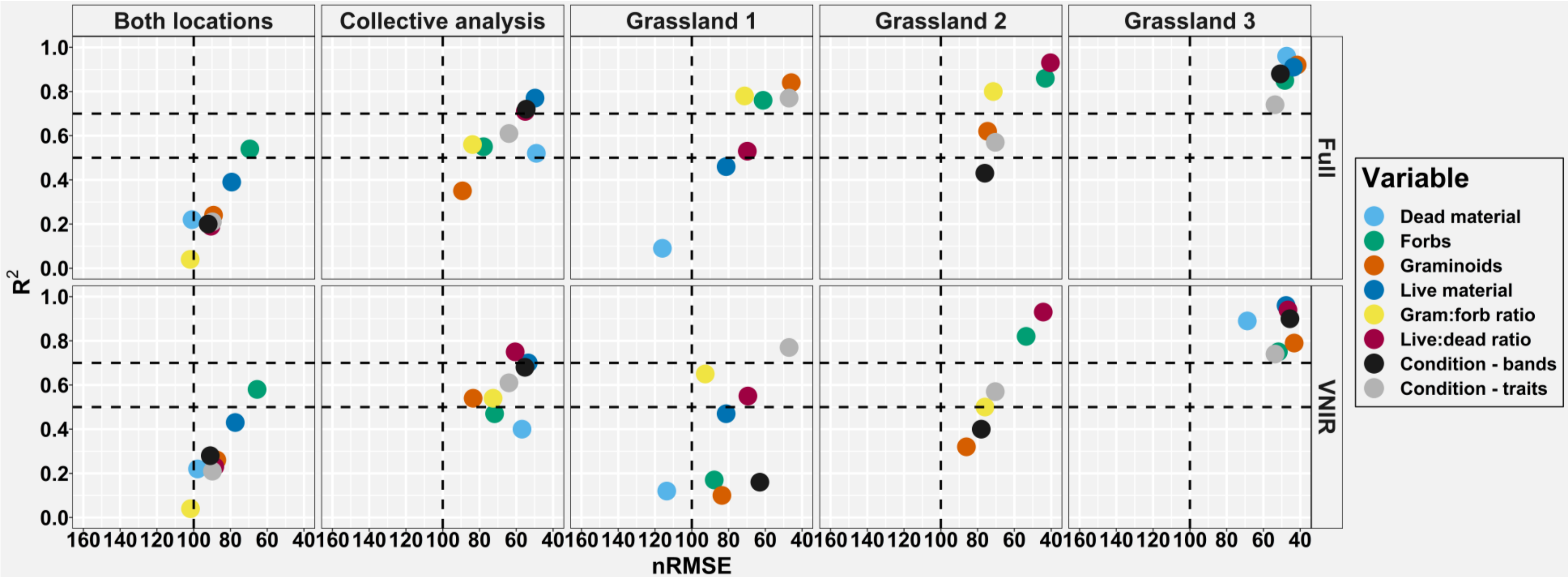

4744

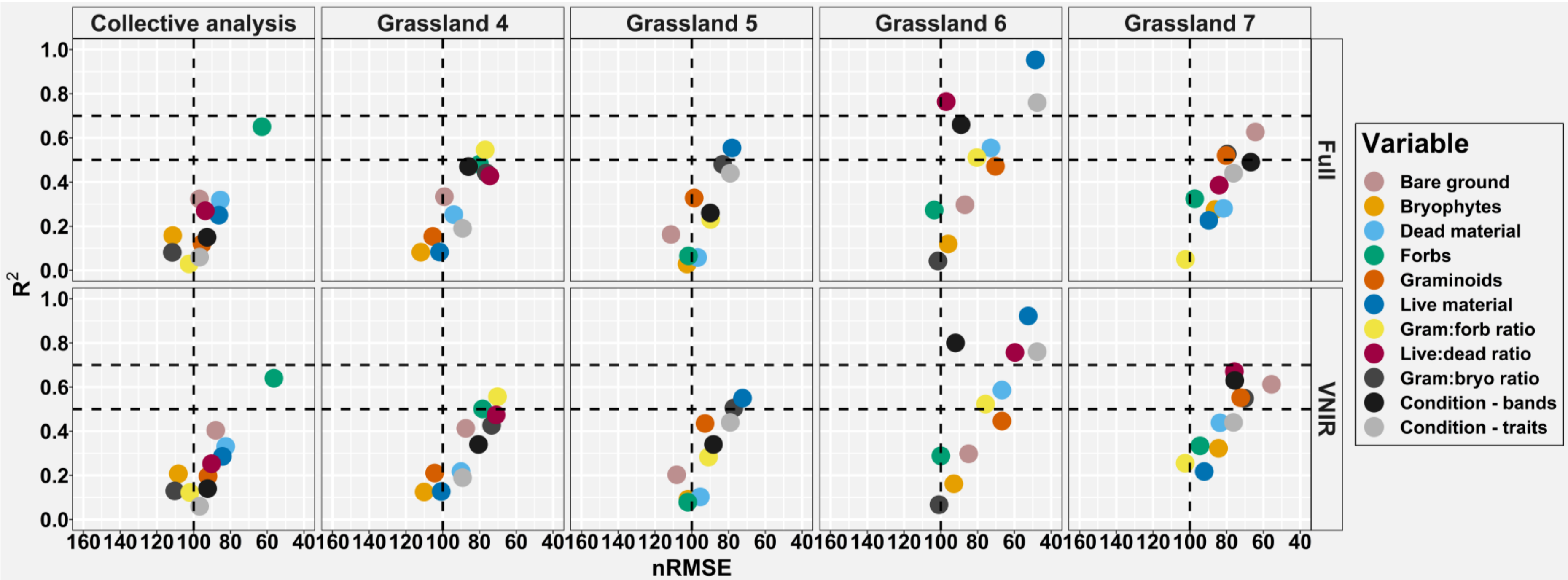
4745



Collective analysis
Grassland 4
Grassland 5
Grassland 6
Grassland 7
Full
VNIR
$R^2$
nRMSE
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Gram:bryo ratio
Condition - bands
Condition - traits

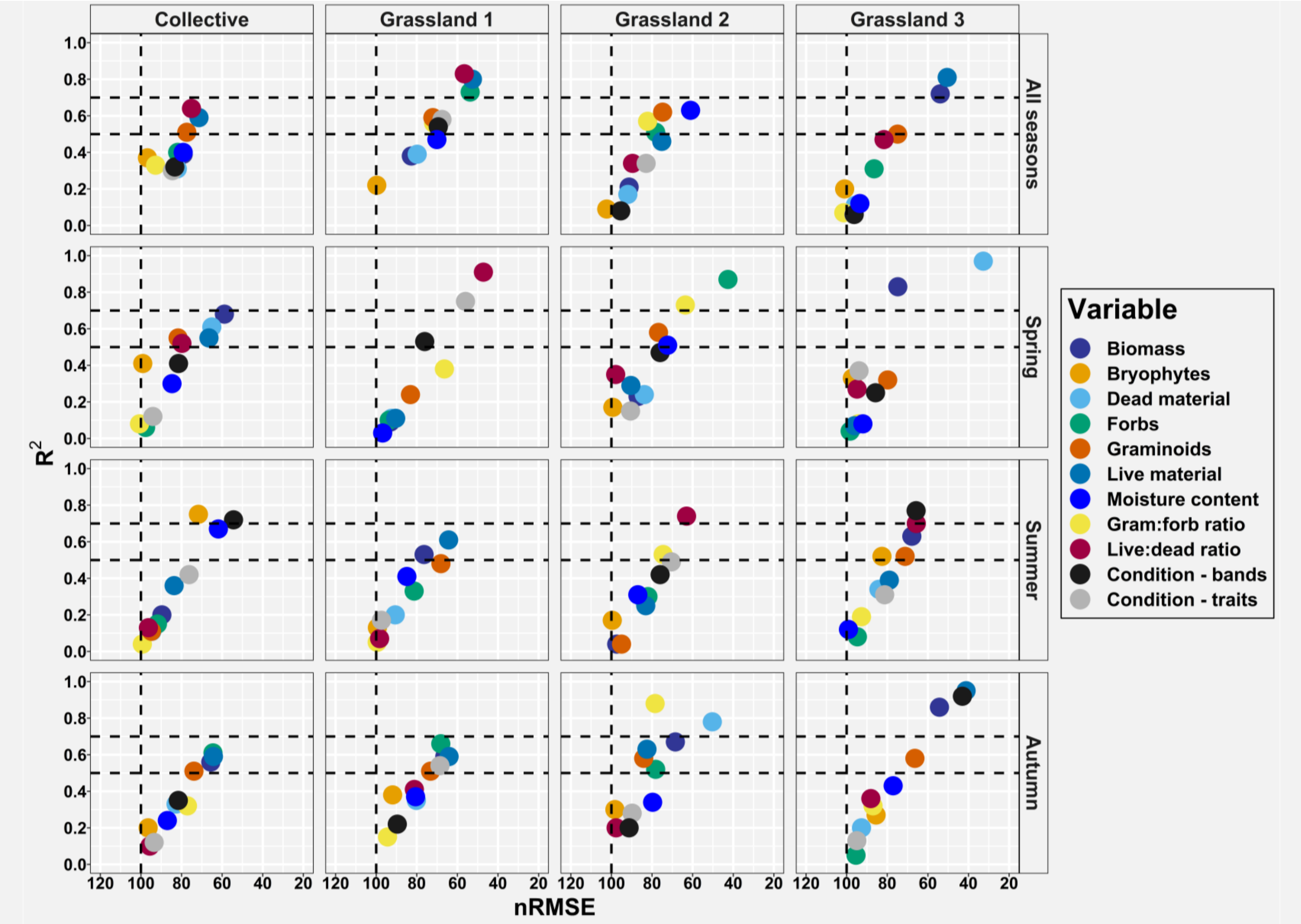

4746


Both locations
Collective analysis
Grassland 1
Grassland 2
Grassland 3
Full
VNIR
$R^2$
nRMSE
1.0
0.8
0.6
0.4
0.2
0.0
160 140 120 100 80 60 40
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

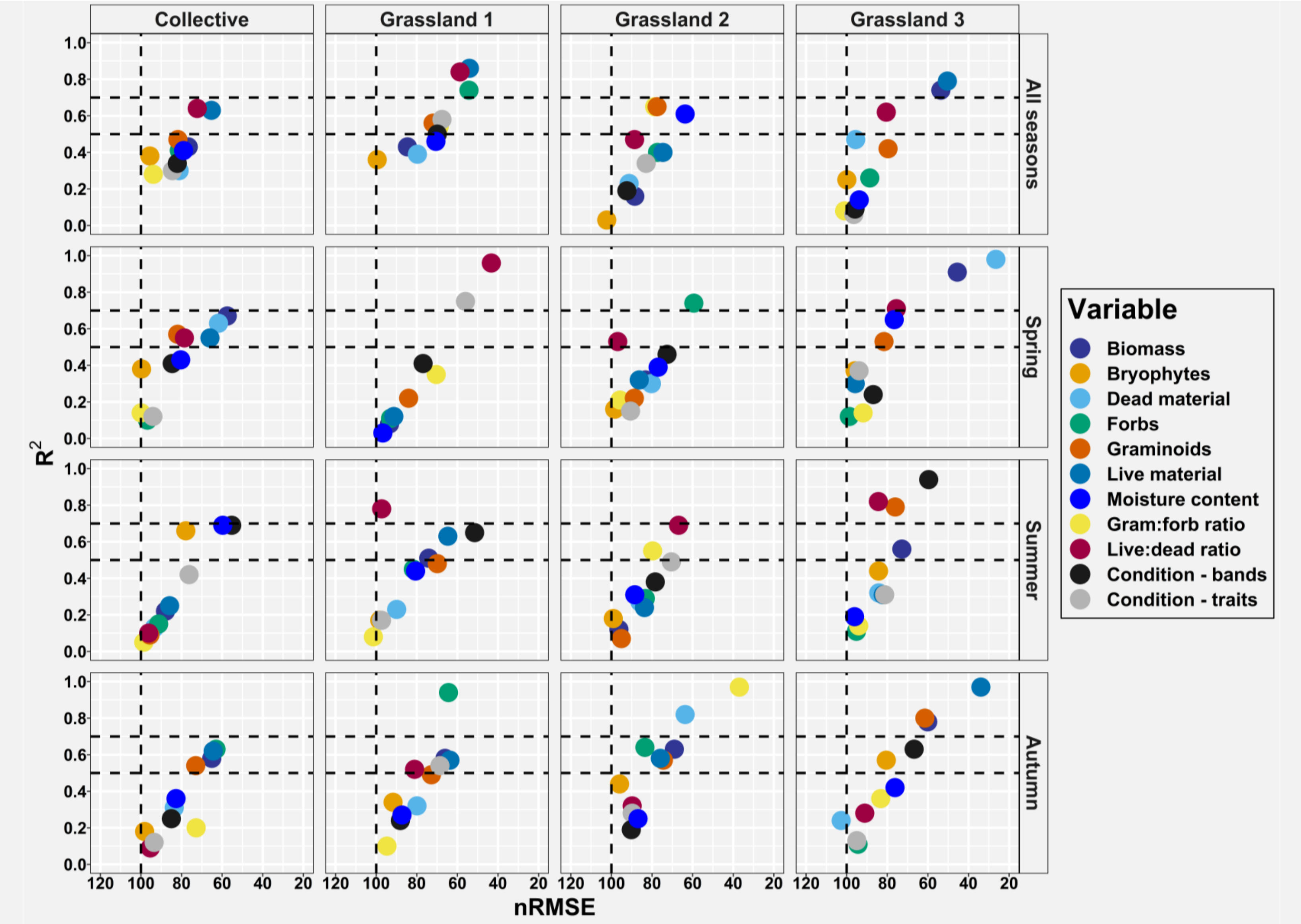



*Appendix Figure 3: Plots for results of 426 PLSR regressions, each of which represent the median* $R^2$ *and nRMSE values of the iterated model runs, where (i) spectral data (either FULL or VNIR) were used to predict grassland variables (coloured dots) and CSM based condition (black dot) and (ii) grassland variables were used to predict CSM based condition (white dot). Panels a and b show results for mass based analysis for Parsonage and Ingleborough respectively, c and d for % cover based analysis for Parsonage and Ingleborough respectively.*

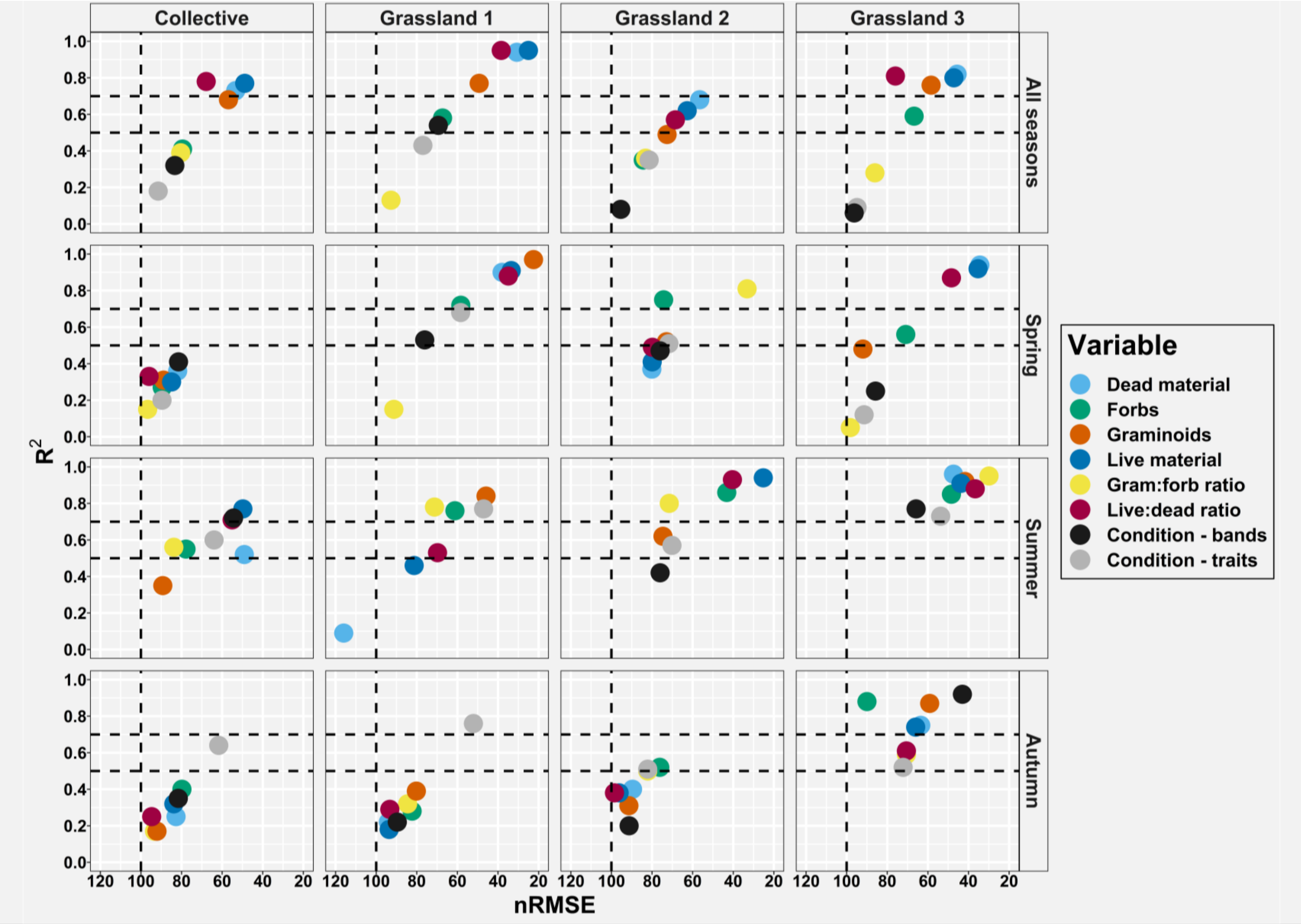
# Chapter 5 full results


Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

4755

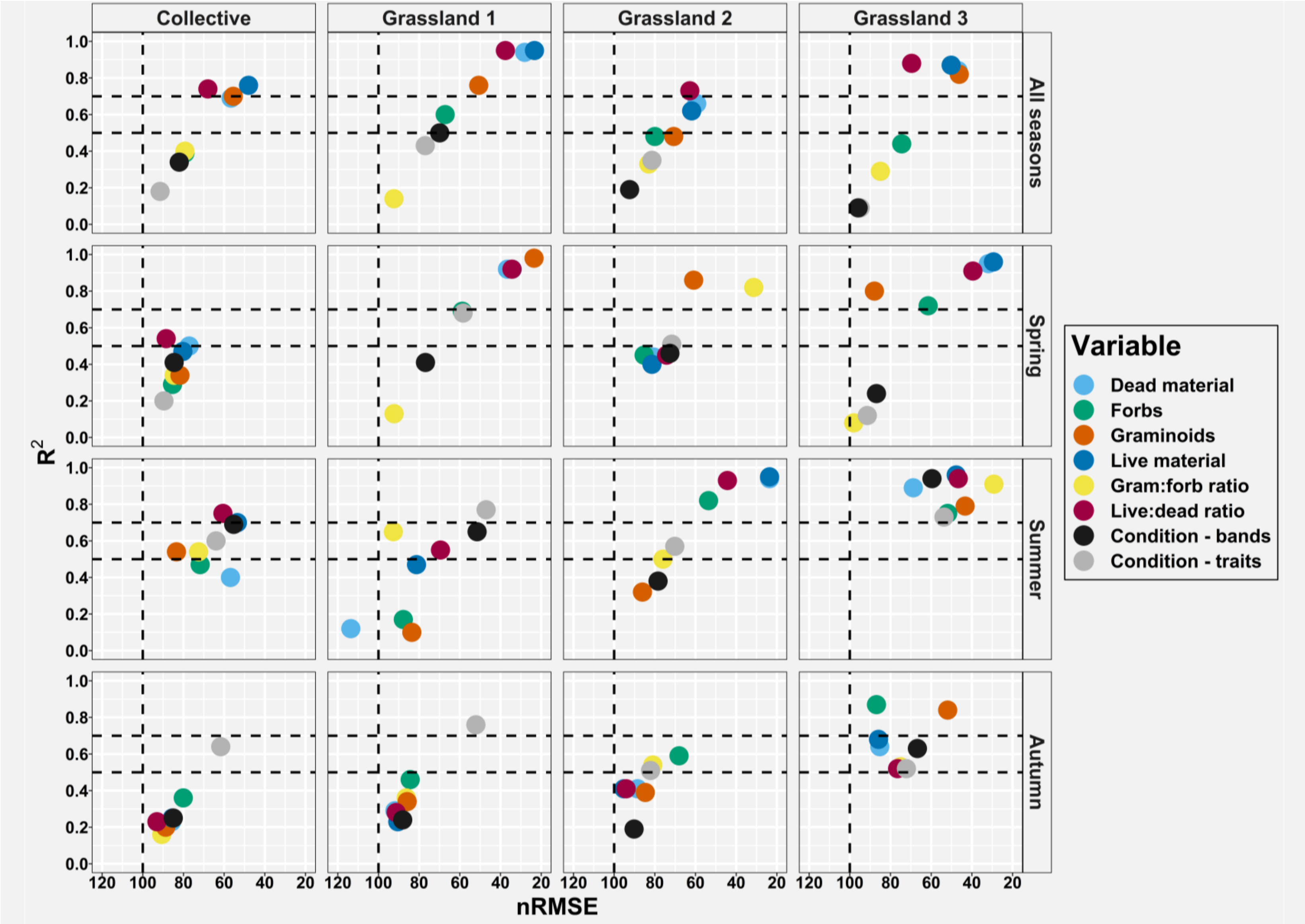

Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
$R^2$
nRMSE
1.0
0.8
0.6
0.4
0.2
0.0
120 100 80 60 40 20
Variable
Biomass
Bryophytes
Dead material
Forbs
Graminoids
Live material
Moisture content
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

4756



Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
1.0
0.8
0.6
0.4
0.2
0.0
120
100
80
60
40
20
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits


4757

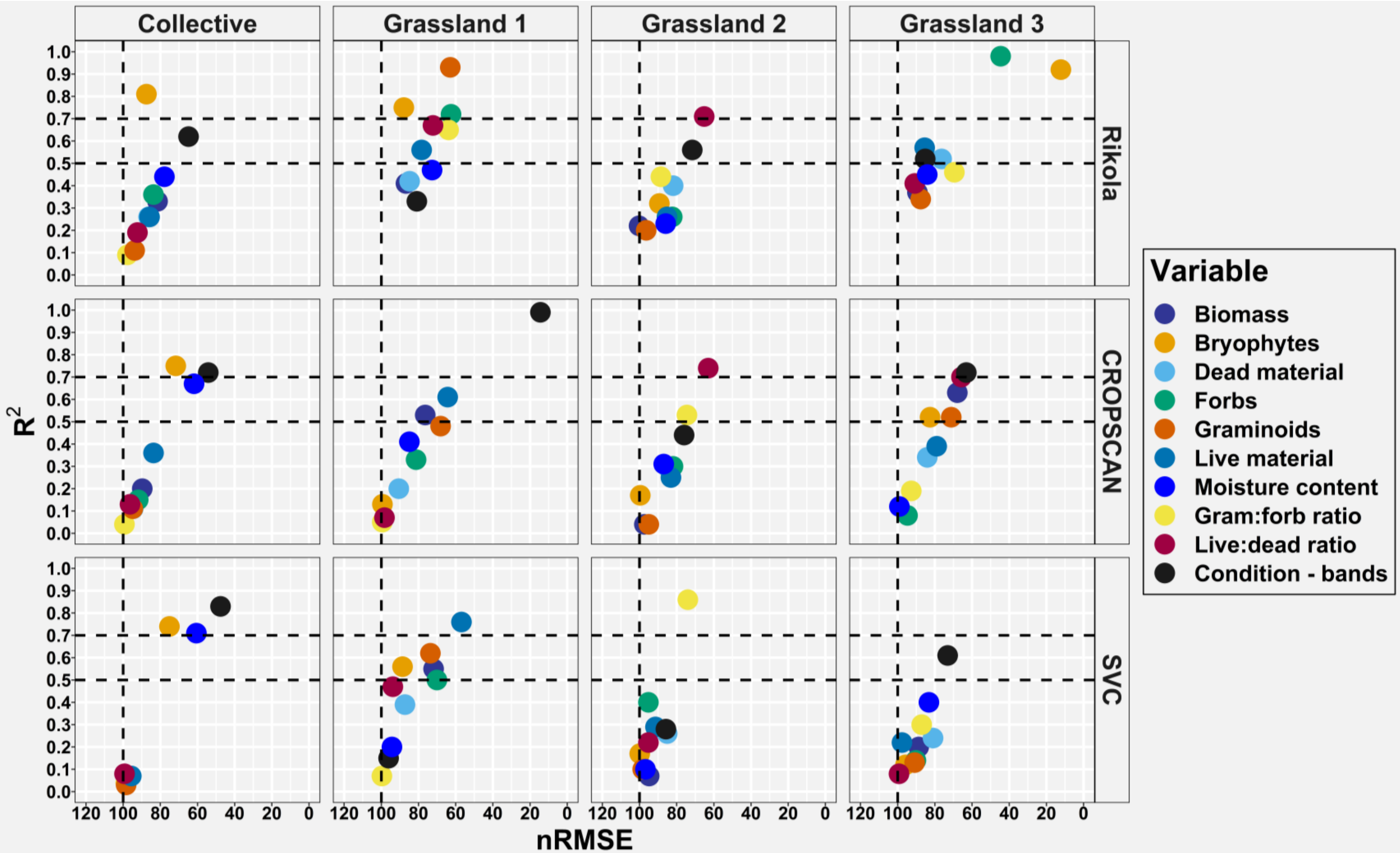


Collective
Grassland 1
Grassland 2
Grassland 3
All seasons
Spring
Summer
Autumn
R2
nRMSE
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio
Condition - bands
Condition - traits

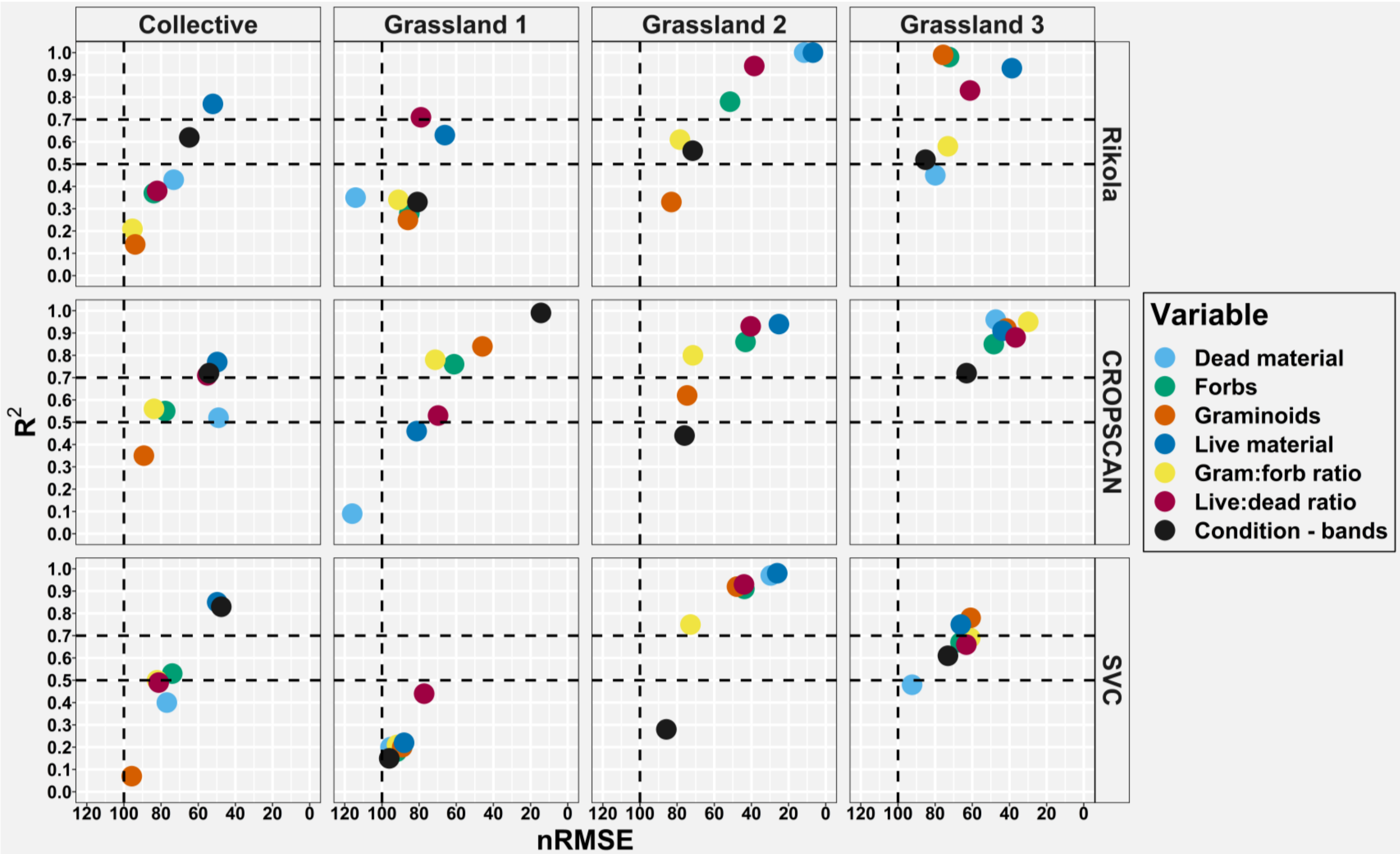

4758

*Appendix Figure 4: Median results of all iterated model runs where spectral data were used to predict CSM-condition and grassland variables for each of the three seasons (n = 10 or 30) and for all seasons (n = 30 or 90). Also included are the results of predicting CSM-condition using grassland variables as predictors. Panels a and b show results for mass based analysis (FULL and VNIR respectively), and panels c and d for % cover based analysis (FULL and VNIR respectively).*

4763 **Chapter 6 full results**

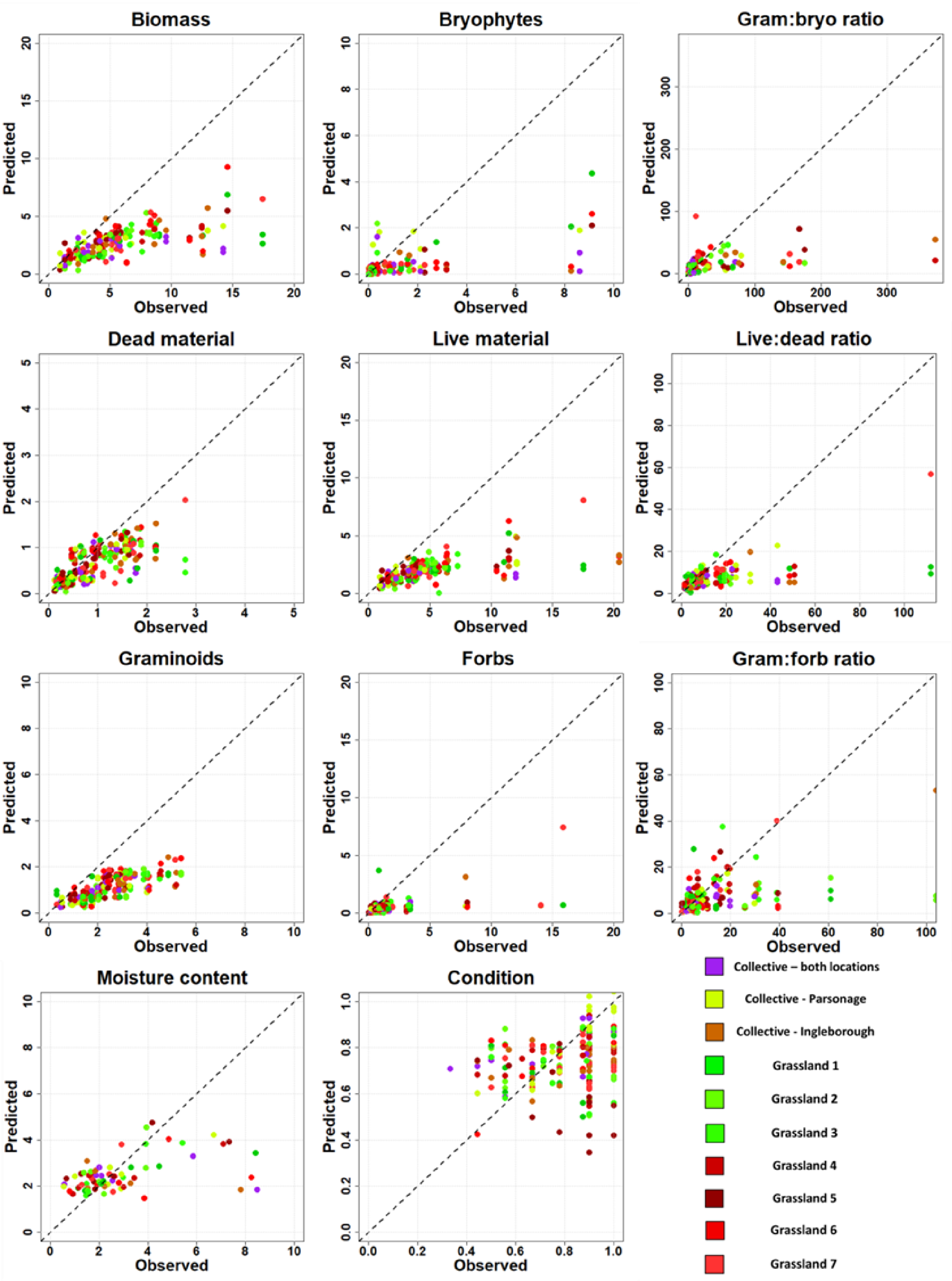


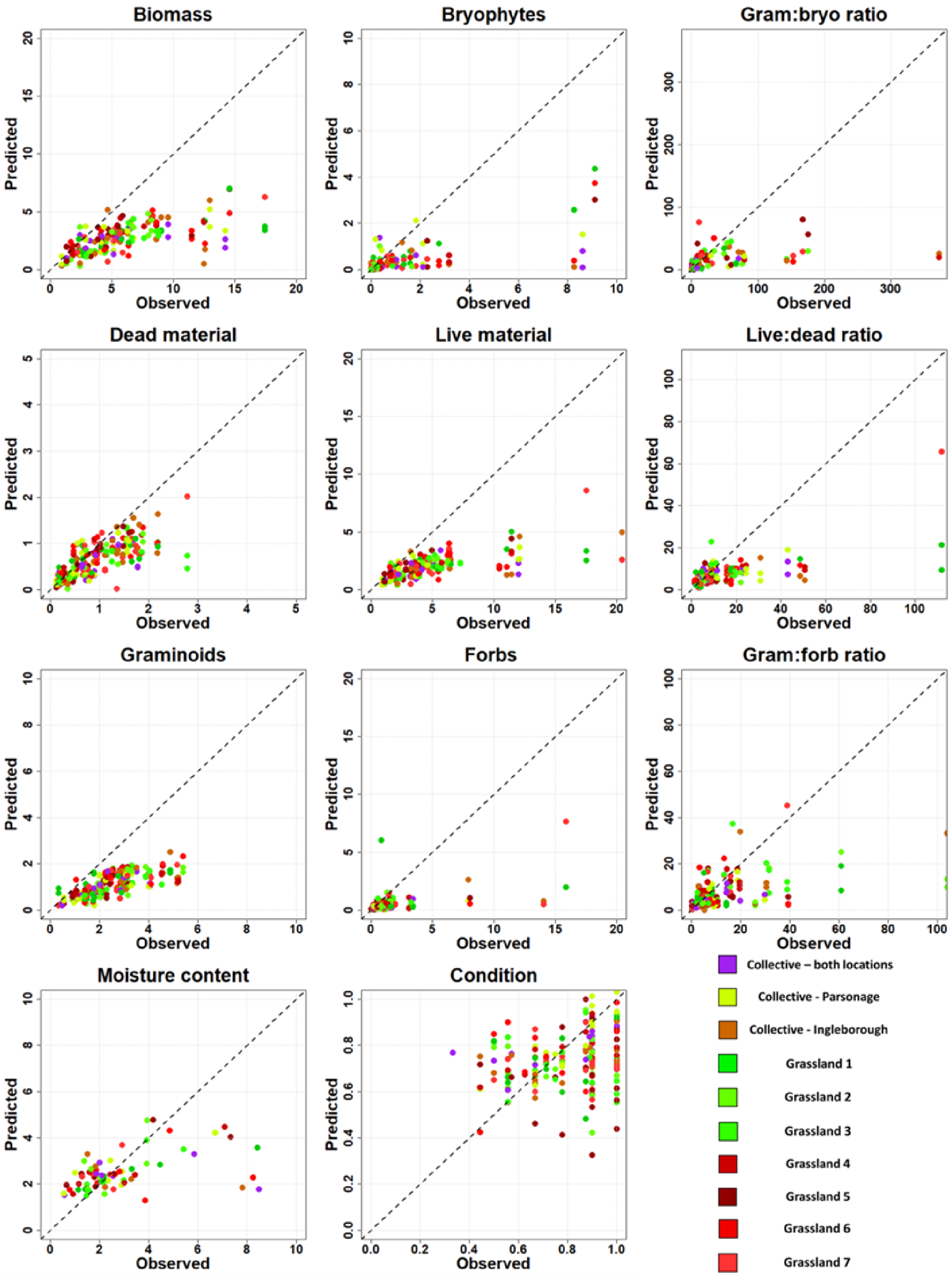

4764


Collective
Grassland 1
Grassland 2
Grassland 3
Rikola
CROPSCAN
SVC
R2
nRMSE
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
120 100 80 60 40 20 0
Variable
Dead material
Forbs
Graminoids
Live material
Gram:forb ratio
Live:dead ratio
Condition - bands

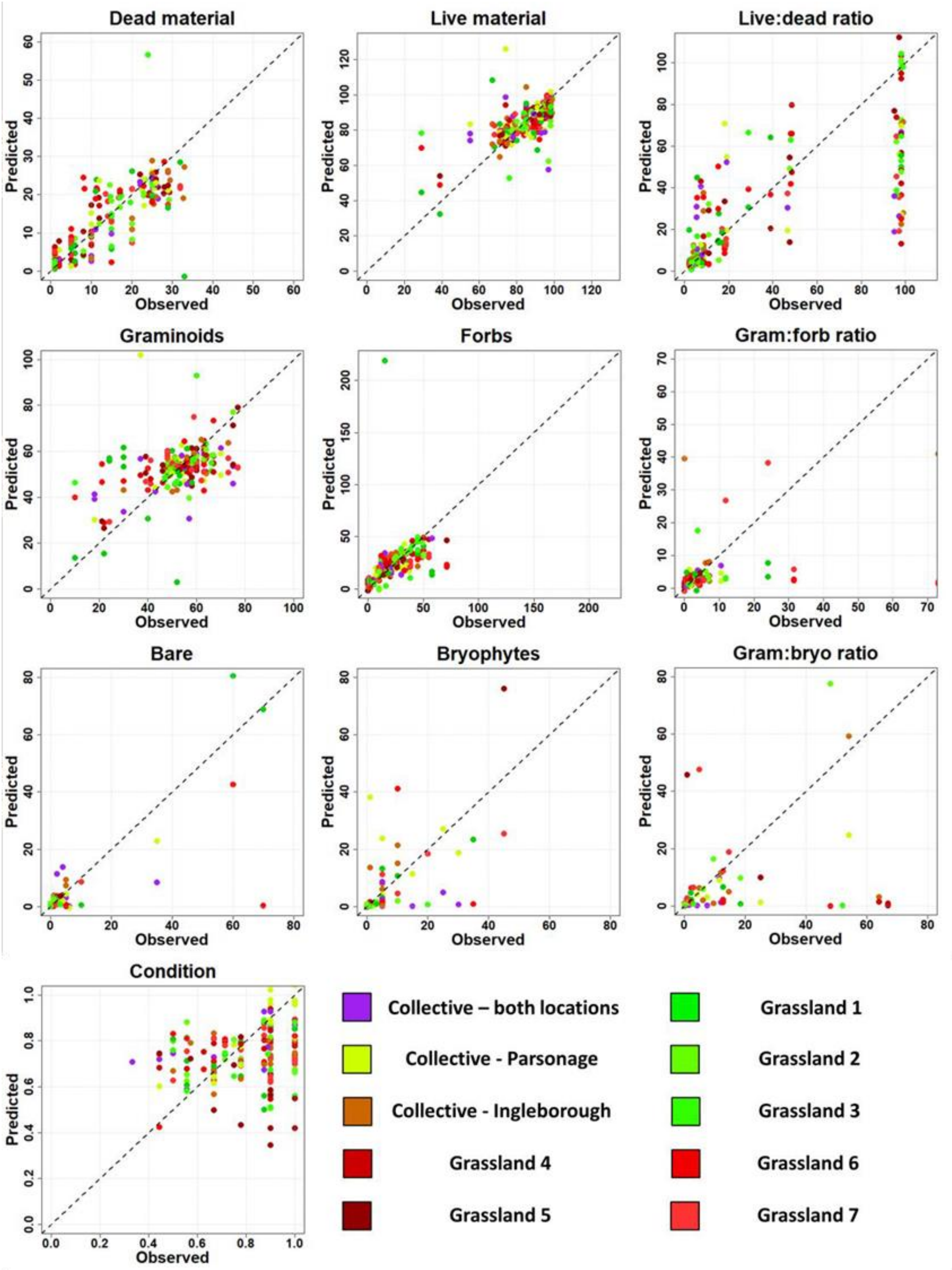
*Appendix Figure 5*: *Median results of iterated model runs where spectral data from three different devices were used to predict grassland variables and CSM-condition for all grasslands collectively (n = 30) or single sites (n = 10). Panel a shows results for mass based analysis and panel b shows results for cover based analysis.*

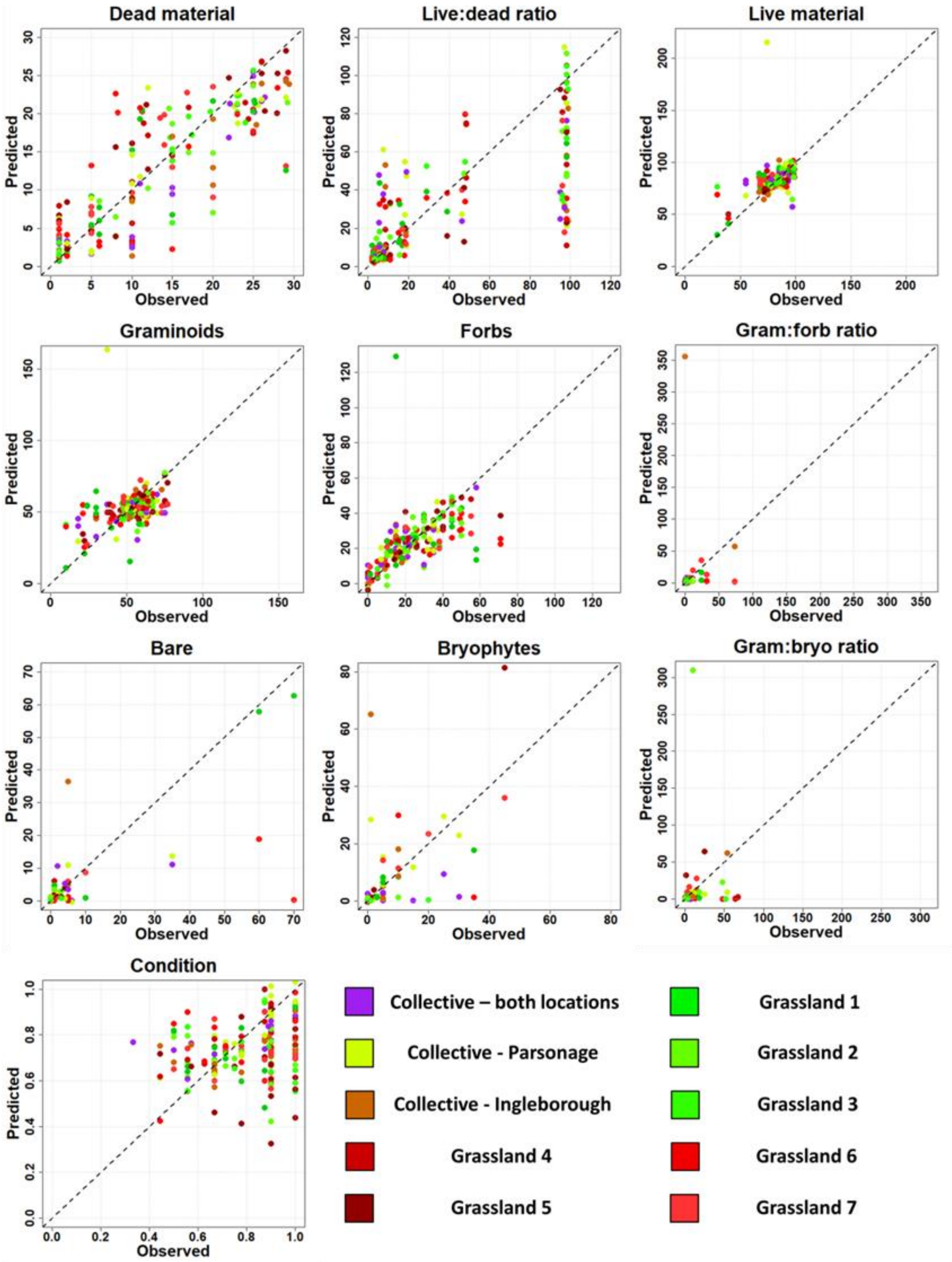
# Observations vs. predictions – Chapter 4





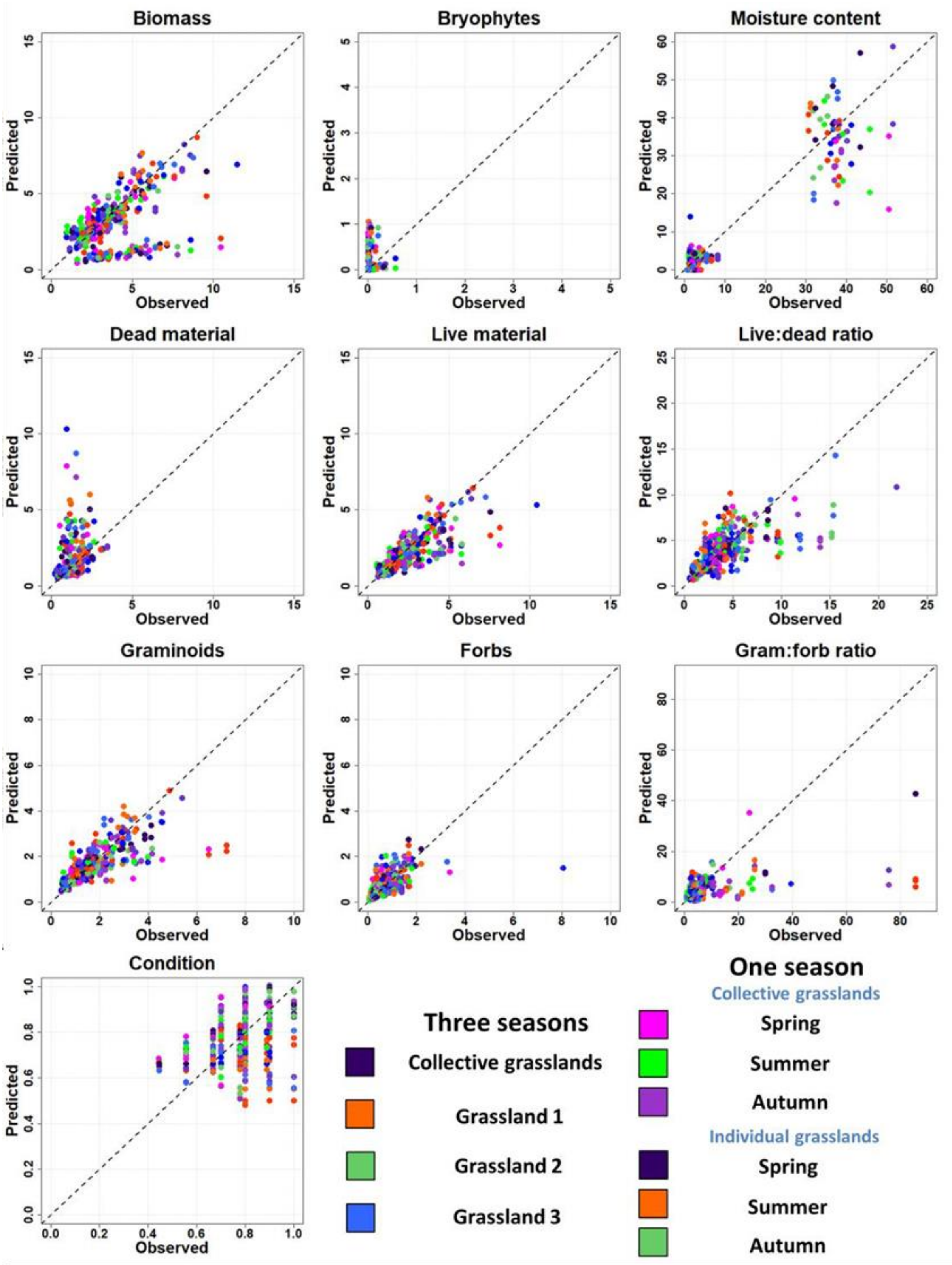
Biomass
Bryophytes
Gram:bryo ratio
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Moisture content
Condition
Predicted
Observed
Collective – both locations
Collective - Parsonage
Collective - Ingleborough
Grassland 1
Grassland 2
Grassland 3
Grassland 4
Grassland 5
Grassland 6
Grassland 7


Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Bare
Bryophytes
Gram:bryo ratio
Condition
Predicted
Observed
Collective – both locations
Collective - Parsonage
Collective - Ingleborough
Grassland 4
Grassland 5
Grassland 1
Grassland 2
Grassland 3
Grassland 6
Grassland 7

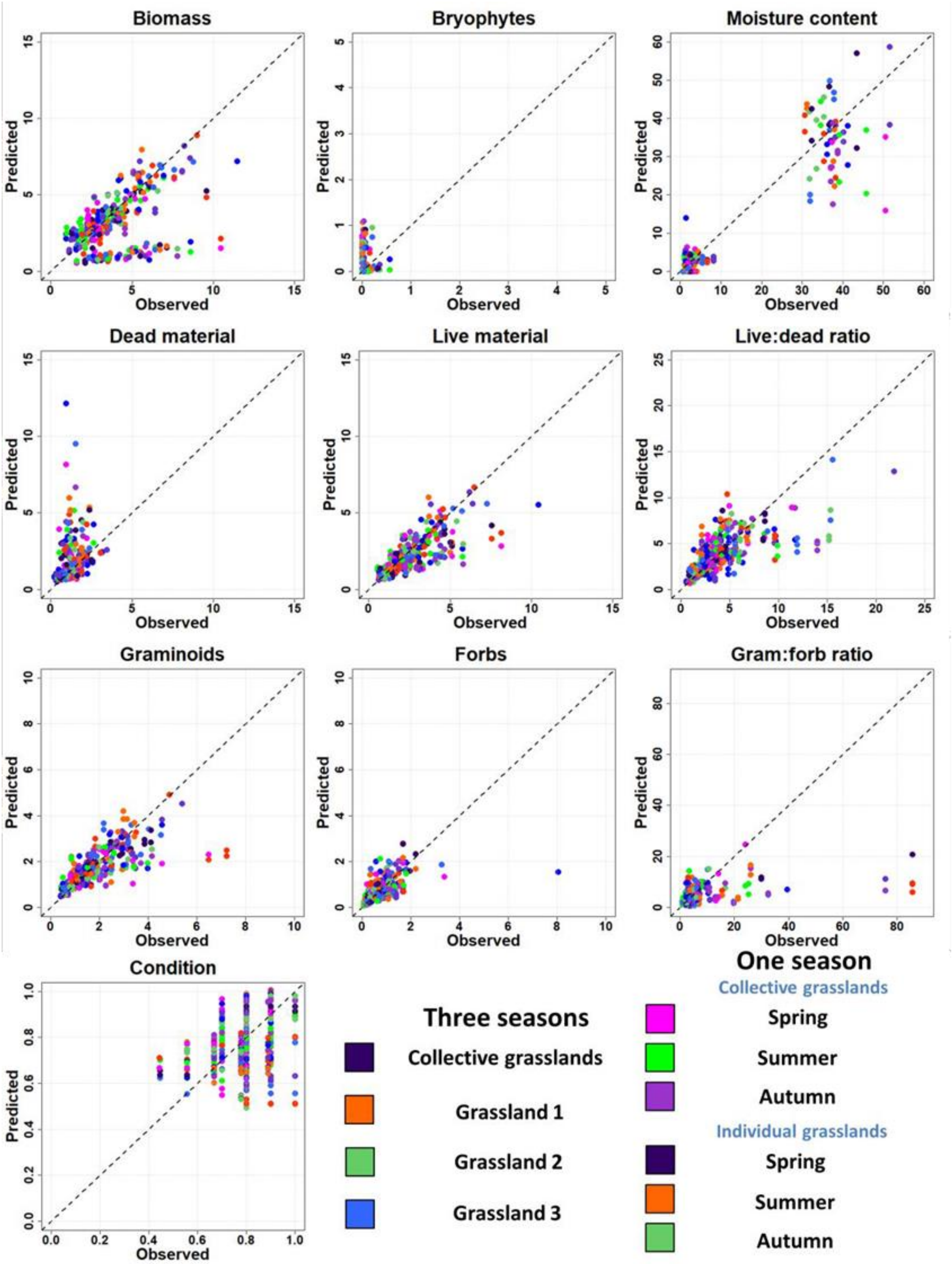


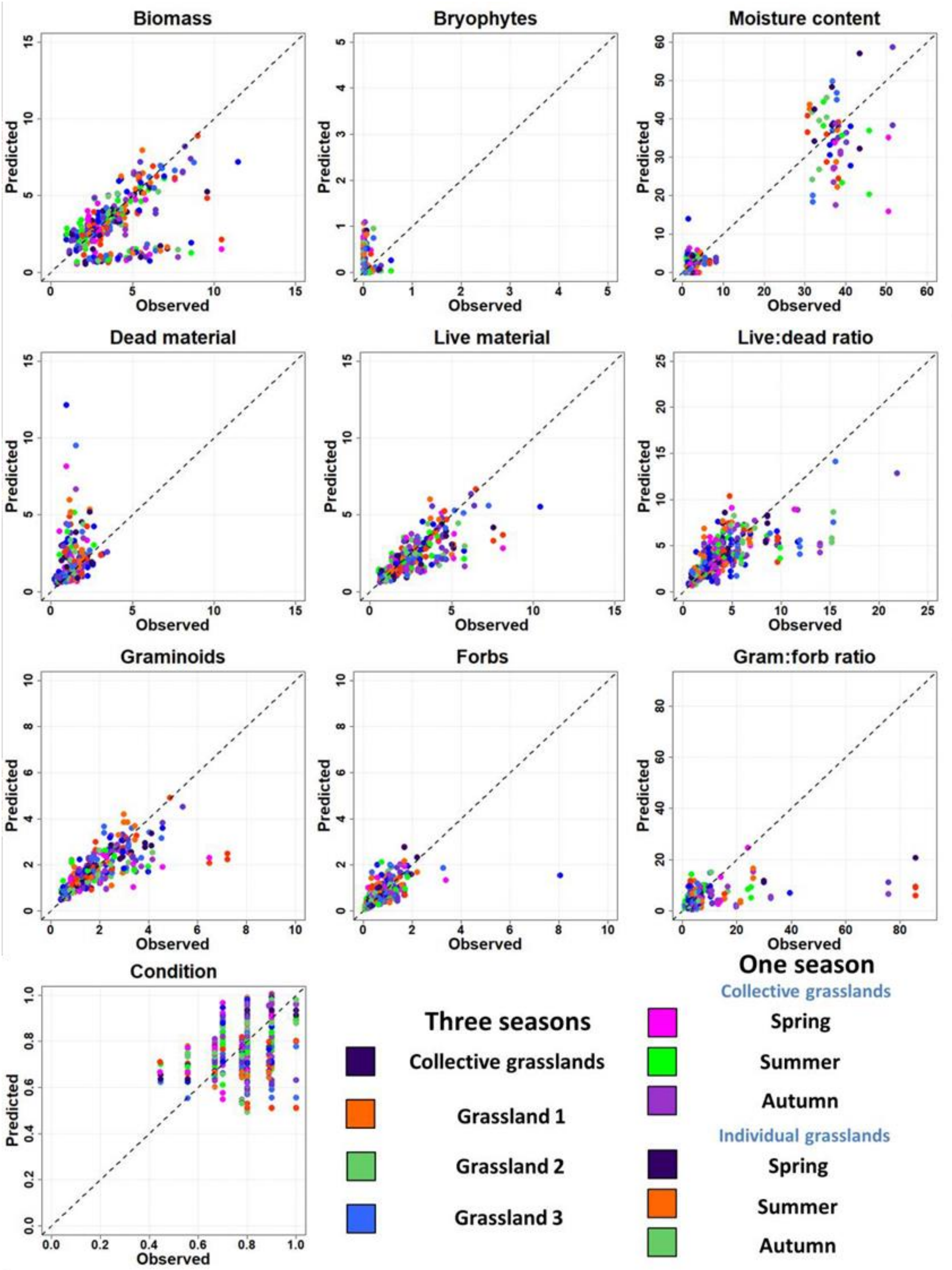

*Appendix Figure 6: Observed and predicted values for each grassland variable and CSM-condition where CROPSCAN spectral data were used as predictors on data collected on all seven grasslands during the summer. The first two sets of graphs project predicted values derived from mass data (except moisture content which is % mass) where the first set are* *the results of using FULL spectral data and the second set of graphs are the result of using VNIR data. The next two sets of graphs are projections of predicted values derived from % cover data, where FULL spectral data and VNIR spectral data were used respectively.*

## Observations vs. predictions – Chapter 5

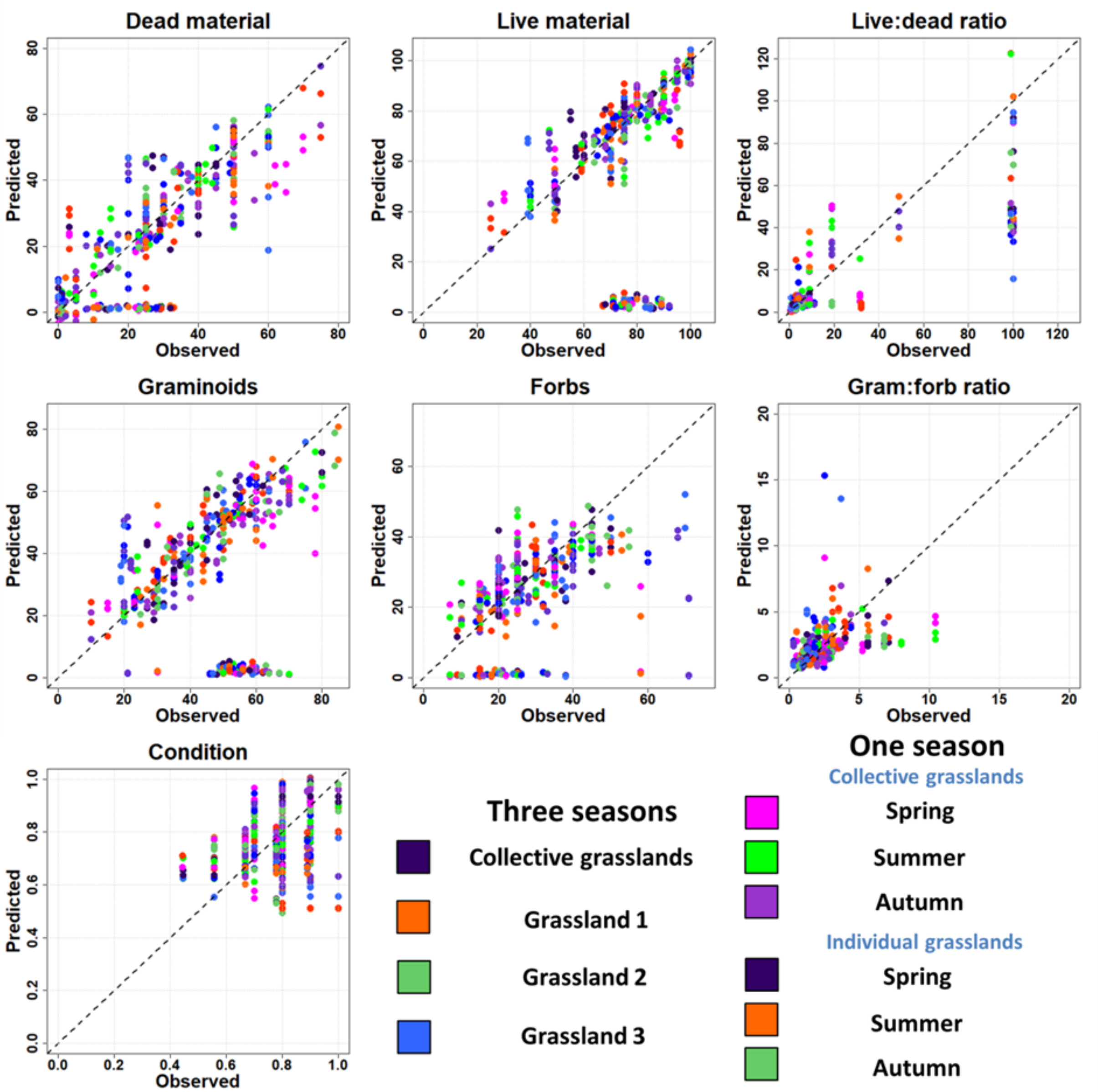


Biomass
Bryophytes
Moisture content
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Condition
Predicted
Observed
Three seasons
Collective grasslands
Grassland 1
Grassland 2
Grassland 3
One season
Collective grasslands
Spring
Summer
Autumn
Individual grasslands
Spring
Summer
Autumn


Biomass
Bryophytes
Moisture content
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Condition
Predicted
Observed
Three seasons
Collective grasslands
Grassland 1
Grassland 2
Grassland 3
One season
Collective grasslands
Spring
Summer
Autumn
Individual grasslands
Spring
Summer
Autumn

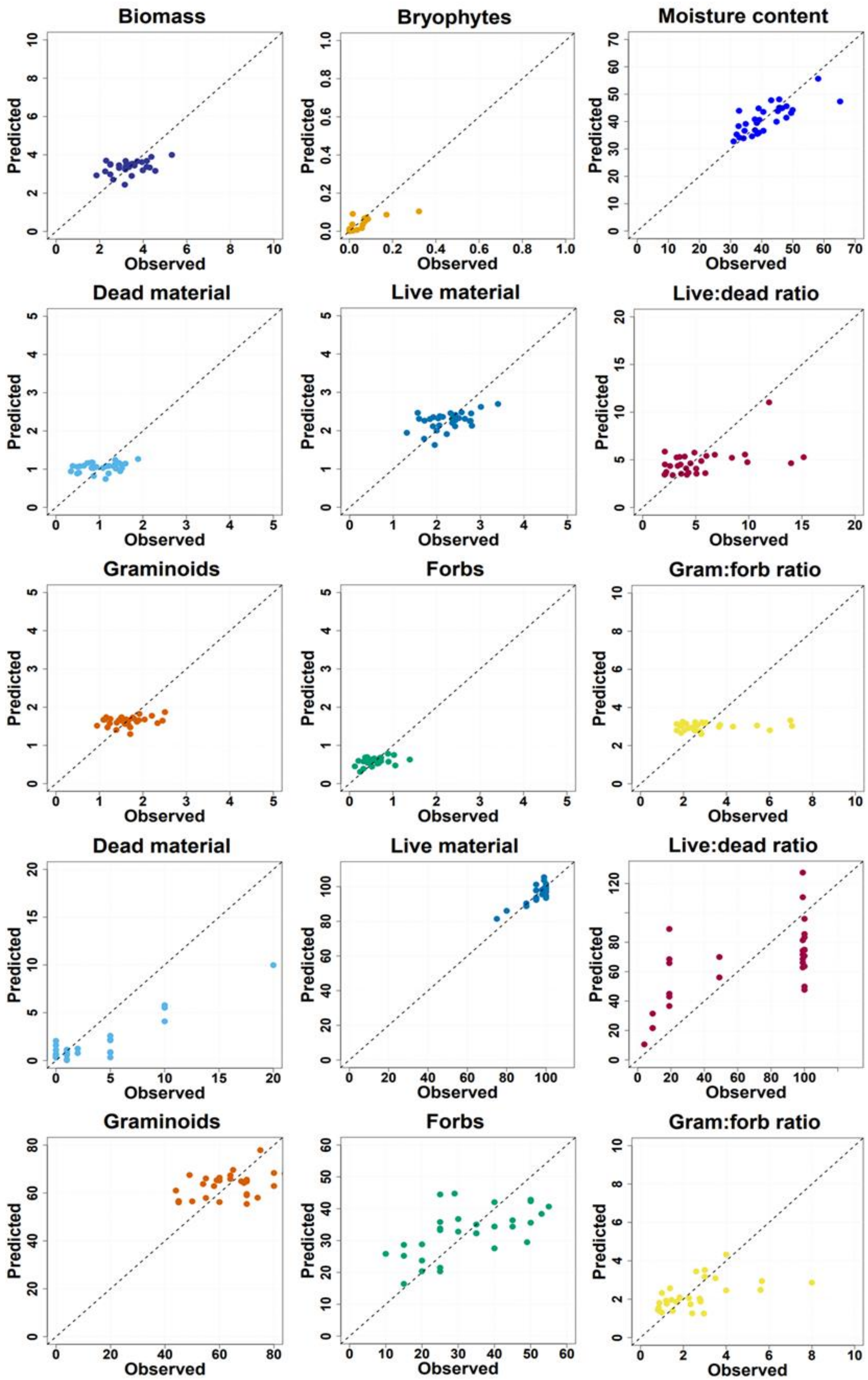


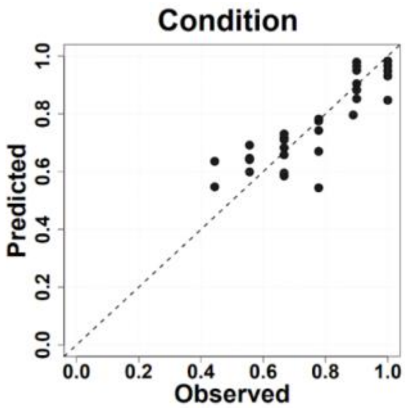
Biomass
Bryophytes
Moisture content
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Condition
Predicted
Observed
Three seasons
Collective grasslands
Grassland 1
Grassland 2
Grassland 3
One season
Collective grasslands
Spring
Summer
Autumn
Individual grasslands
Spring
Summer
Autumn



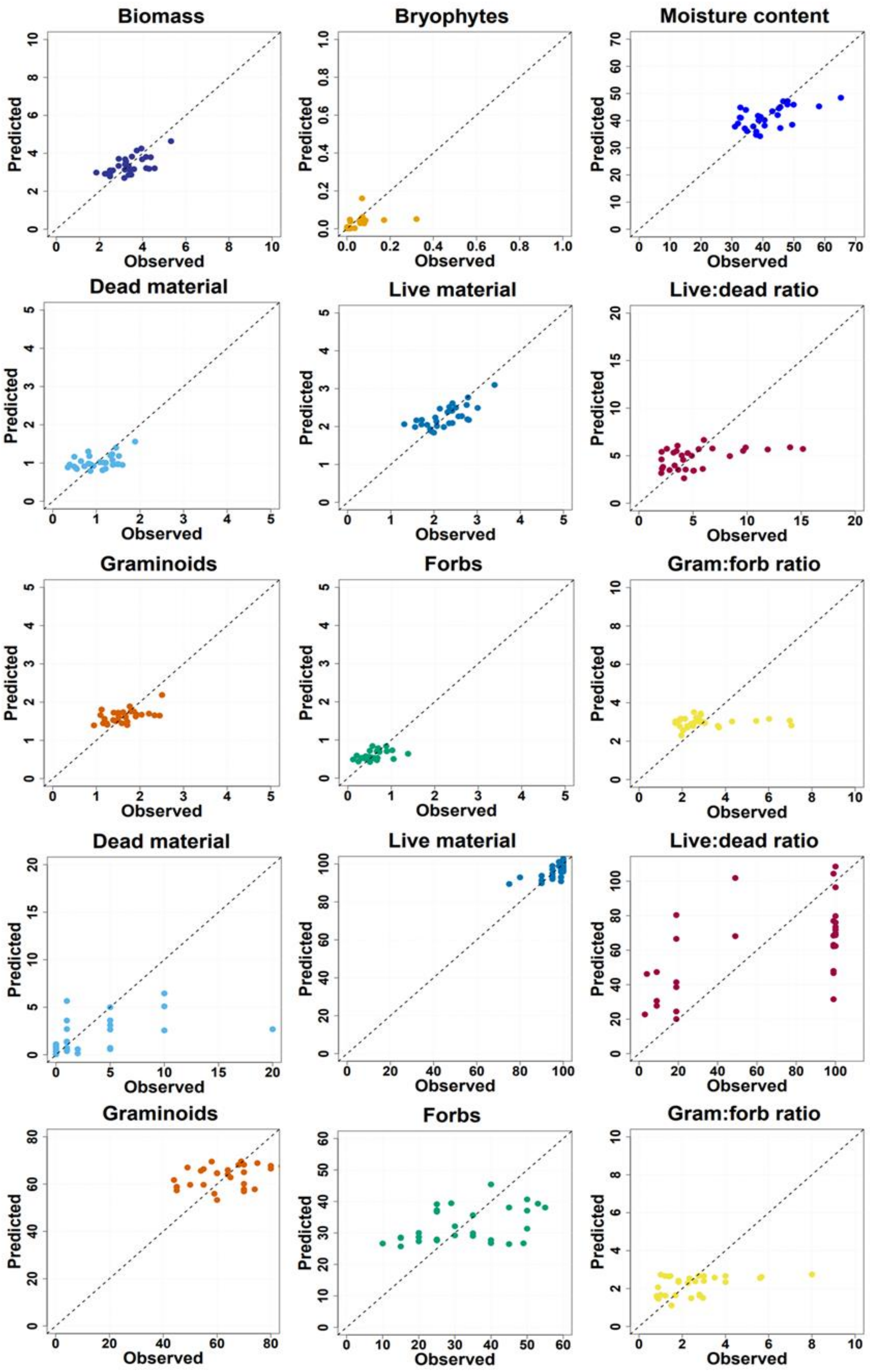

Appendix Figure 7: Observed and predicted values for each grassland variable and CSM-condition where CROPSCAN spectral data were used as predictors on data collected over three seasons on Parsonage grasslands. The first two sets of graphs project predicted values derived from mass data (except moisture content which is % mass) where the first set are the results of using FULL spectral data and the second set of graphs are the result of using VNIR data. The next two sets of graphs are projections of predicted values derived from % cover data, where FULL spectral data and VNIR spectral data were used respectively. The data sets used include data collected on all three grasslands across three seasons, on one grassland across three seasons, across all grasslands for one season and on one grassland for one season.

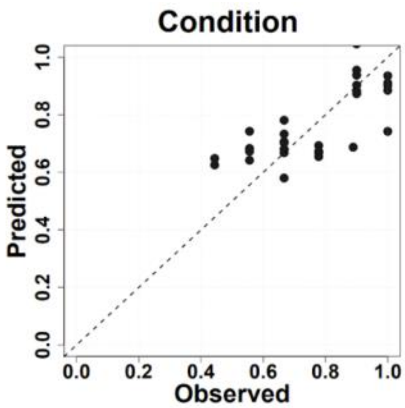
## Observations vs. predictions – Chapter 6


Biomass
Bryophytes
Moisture content
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Predicted
Observed



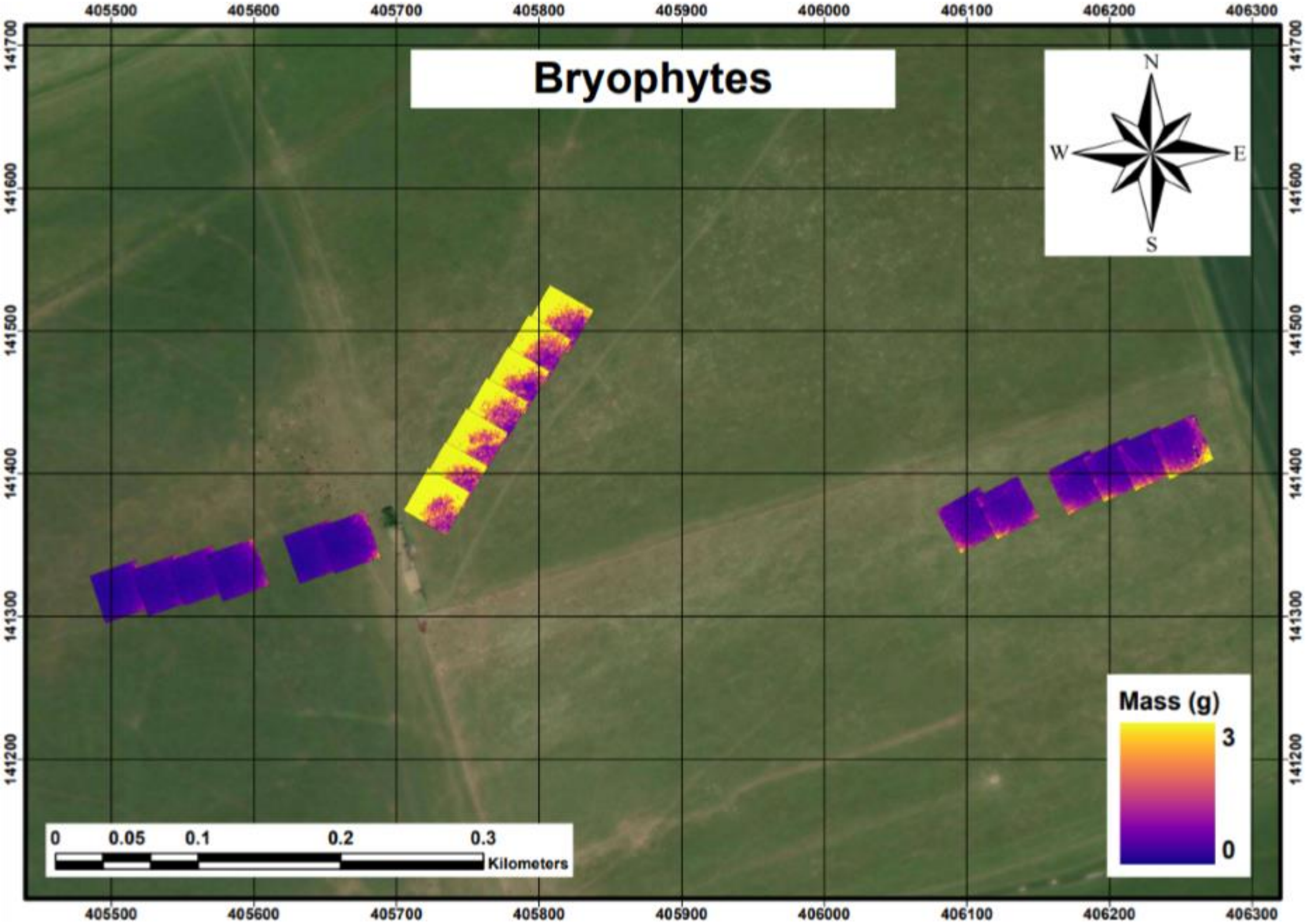

*Appendix Figure 7: Observed and predicted values for each grassland variable and CSM-condition where CROPSCAN spectral data were used as predictors. The first three rows project predicted values derived from mass data (except moisture content which is % mass) and the bottom two rows project predicted values derived from % cover data.*


Biomass
Bryophytes
Moisture content
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Dead material
Live material
Live:dead ratio
Graminoids
Forbs
Gram:forb ratio
Predicted
Observed



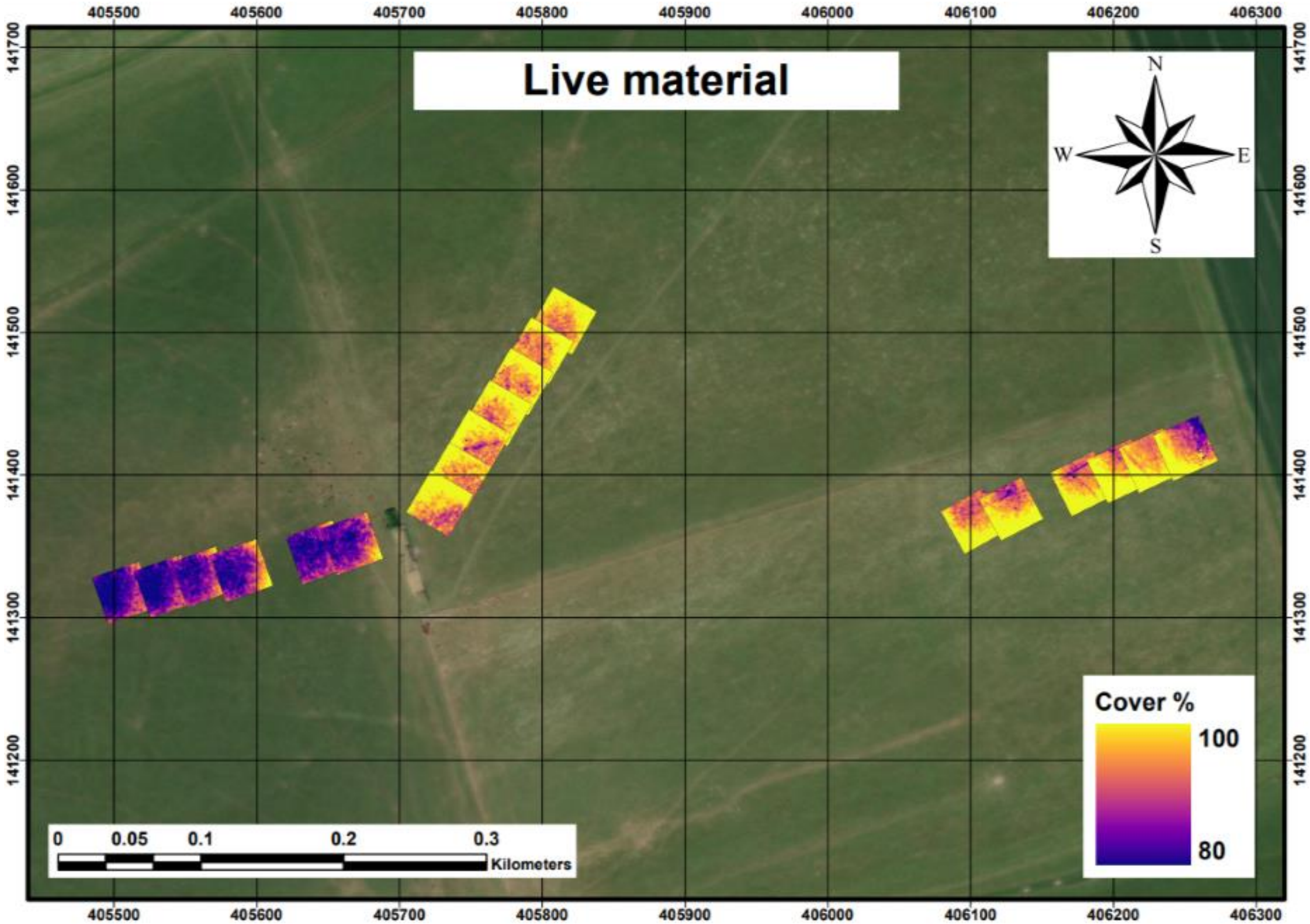

*Appendix Figure 8: Observed and predicted values for each grassland variable and CSM-condition where Rikola spectral data were used as predictors. The first three rows project predicted values derived from mass data (except moisture content which is % mass) and the penultimate two rows project predicted values derived from % cover data. The bottom projection shows predicted values for CSM-condition.*

## Extrapolating predicted grassland variables and condition using Rikola data as predictors

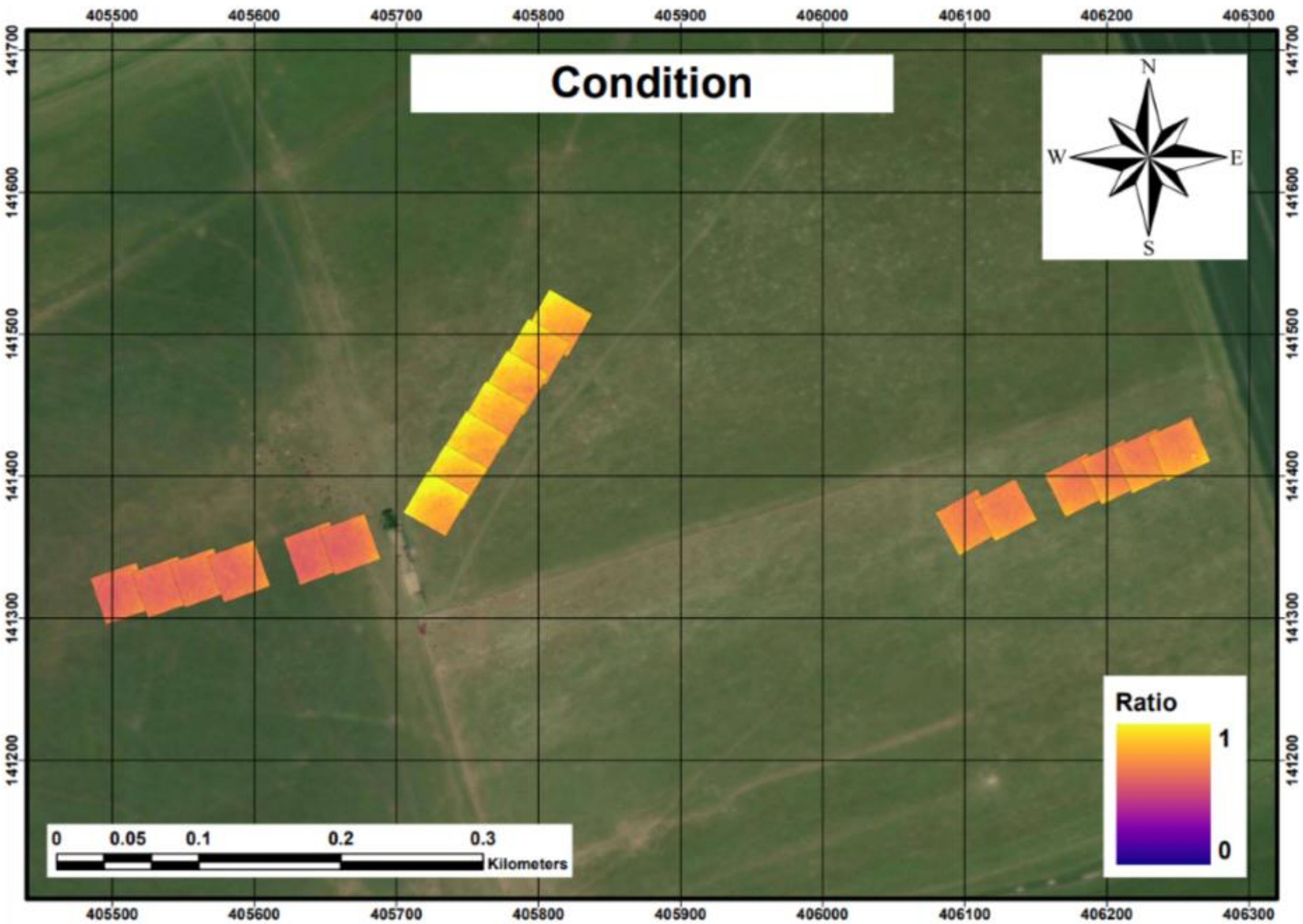



4833

4834 Appendix Figure 4a: Projection of predicted bryophyte mass predicted values derived from a PLSR model trained with Rikola data.




Appendix Figure 4b: Projection of predicted live material % cover predicted values derived from a PLSR model trained with Rikola data.




Appendix Figure 4c: Projection of ‘condition’ predicted values derived from a PLSR model trained with Rikola data.